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NEWS	1			Web Page for STN Seminar Schedule - N. America
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				and Japanese-language basic patents from 2004-present
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NEWS	6	DEC	01	ChemPort single article sales feature unavailable
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				coverage of complete UK patent families
NEWS	8	DEC	17	Fifty-one pharmaceutical ingredients added to PS
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NEWS	10	JAN	07	WPIDS, WPINDEX, and WPIX enhanced Japanese Patent
				Classification Data
NEWS	11	FEB	02	Simultaneous left and right truncation (SLART) added
				for CERAB, COMPUAB, ELCOM, and SOLIDSTATE
NEWS	12	FEB	02	GENBANK enhanced with SET PLURALS and SET SPELLING
NEWS	13	FEB	06	Patent sequence location (PSL) data added to USGENE
NEWS	14	FEB	10	COMPENDEX reloaded and enhanced
NEWS		FEB		WTEXTILES reloaded and enhanced
NEWS	16	FEB	19	New patent-examiner citations in 300,000 CA/CAplus
				patent records provide insights into related prior
				art
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NEWS	18	FEB	23	Several formats for image display and print options
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NEWS	19	FEB	23	MEDLINE now offers more precise author group fields
				and 2009 MeSH terms
NEWS	20	FEB	23	TOXCENTER updates mirror those of MEDLINE - more
				precise author group fields and 2009 MeSH terms
NEWS	21	FEB	23	Three million new patent records blast AEROSPACE into
				STN patent clusters
NEWS	22	FEB	25	USGENE enhanced with patent family and legal status
				display data from INPADOCDB
NEWS	23	MAR	06	INPADOCDB and INPAFAMDB enhanced with new display
				formats
NEWS	24	MAR	11	EPFULL backfile enhanced with additional full-text
				applications and grants
NEWS	25	MAR	11	ESBIOBASE reloaded and enhanced
NEWS	EXPI	RESS		E 27 08 CURRENT WINDOWS VERSION IS V8.3,
			AND	CURRENT DISCOVER FILE IS DATED 23 JUNE 2008.

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N.N-DIMETHYLETHYLENEDIAMINE DIPROTONATED/CN

http://www.cas.org/support/stngen/stndoc/properties.html

=> e N.N-dimethvlethanolammonium formate/cn E1 N.N-DIMETHYLETHANOLAMINOGALLANE DIMER/CN E2 N, N-DIMETHYLETHANOLAMMONIUM/CN E3 0 --> N,N-DIMETHYLETHANOLAMMONIUM FORMATE/CN Ε4 1 N, N-DIMETHYLETHENESULFONAMIDE/CN E5 1 N, N-DIMETHYLETHYLAMINE/CN N,N-DIMETHYLETHYLAMINE ALANE/CN N,N-DIMETHYLETHYLAMINE HYDRIODIDE/CN N,N-DIMETHYLETHYLAMINE HYDROCHLORIDE/CN E6 E7 E8 1 E9 1 N, N-DIMETHYLETHYLENEDIAMINE/CN E10 1 N,N-DIMETHYLETHYLENEDIAMINE CYCLIC UREA/CN 1 N,N-DIMETHYLETHYLENEDIAMINE DIHYDROCHLORIDE/CN E11

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E1
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                  N.N-DIMETHYLETHANOLAMINIC METHACRYLATE-TRIMETHYLOLPROPANE TR
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E2
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    36833-64-4 REGISTRY
RN
ED
    Entered STN: 16 Nov 1984
    Ethanol, 2-(dimethylamino)-, conjugate acid (1:1) (CA INDEX NAME)
OTHER CA INDEX NAMES:
    Ethanol, 2-(dimethylamino)-, conjugate monoacid (9CI)
OTHER NAMES:
CN
    2-(N,N-Dimethylamino)ethanol conjugate acid
CN
    N,N-Dimethyl-2-hydroxyethylammonium cation
CN
   N.N-Dimethvlethanolammonium
   C4 H11 N O . H
MF
LC
    STN Files: CA, CAPLUS, TOXCENTER, USPATFULL
CRN (108-01-0)
Me2N-CH2-CH2-OH
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              15 REFERENCES IN FILE CA (1907 TO DATE)
              3 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
              16 REFERENCES IN FILE CAPLUS (1907 TO DATE)
=> file caplus;s us20070185330/pn
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FULL ESTIMATED COST
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This file contains CAS Registry Numbers for easy and accurate substance identification.

1 US20070185330/PN 1.2

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- ANSWER 1 OF 1 CAPLUS COPYRIGHT 2009 ACS on STN
- 2005:1090138 CAPLUS AN
- DN 143:386681
- ED Entered STN: 12 Oct 2005
- TI Ionic liquids containing protonated primary, secondary or tertiary ammonium ions
- IN Walker, Adam John
- PA The University of York, UK
- SO Brit. UK Pat. Appl., 62 pp.
- CODEN: BAXXDU
- Patent DT
- LA English
- IC ICM C07C215-08
- ICS C07C215-12; C07C217-30
- 23-4 (Aliphatic Compounds)
- Section cross-reference(s): 45 EAN ONT 1

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EP 1805131
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    MX 2006011531
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    KR 2007031302
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WO 2005-GB1364
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CLASS
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KR 2007031302 IPCI C07C0215-40 [I,A]; C07C0215-00 [I,A]
US 20070185330 IPCI C07C0215-02 [I,A]; C07C0215-00 [I,C*]; C07D0211-02
                       [I,A]; C07D0211-00 [I,C*]
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- OS MARPAT 143:386681
- AB The present invention relates to ionic ligs. comprising an anion and a cation wherein the cation is a primary, secondary or tertiary ammonium ion containing a protonated nitrogen atom. The invention also provides processes for the manufacture of ionic ligs. For example, N. N-dimethylethanolammonium glycolate (1) was prepared by gradually adding glycolic acid to an alc. solution of N.N-dimethylethanolamine; after completion and neutralization, the cold alc. solution was filtered, solvent removed, then frozen in liquid nitrogen and lyophilized in vacuo. After gradually allowing the sample to warm to room temperature, 32.85 g (93% yield) of I as a pale yellow liquid was isolated. Preferred ionic ligs. contain ethanolammonium, diethanolammonium, N-butyldiethanolammonium, N.N-dimethylethanolammonium, N-methylethanolammonium, N.M-dimethylethanolammonium, N.M-dimethylethanolamm
 - 1-(3-hydroxypropyl)putrescinium ions as cations.
 - T amine acid; ammonium ionic liq prepn; primary ammonium ion prepn ionic liq; secondary ammonium ion prepn ionic liq; tertiary ammonium ion prepn ionic liq
- IT Oxidation

(enzymic; demonstration of application of ionic liqs. in enzymic oxidation
of methanol to formaldehyde)

IT Green chemistry Ionic liquids

(preparation and methods for manufacture of ionic liqs. containing protonated

primary, secondary or tertiary ammonium ions)

IT Quaternary ammonium compounds, preparation

RL: IMF (Industrial manufacture); NUU (Other use, unclassified); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)

(preparation and methods for manufacture of ionic liqs. containing protonated $% \left(1\right) =\left(1\right) \left(1\right) \left($

primary, secondary or tertiary ammonium ions)

IT Acids, reactions

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation and methods for manufacture of ionic liqs. containing protonated

primary, secondary or tertiary ammonium ions)

IT Solvents

 $% \left(\mathcal{G}_{1}\right) =\left(\mathcal{G}_{1}\right)$ (preparation and methods for manufacture of ionic liqs. containing protonated

primary, secondary or tertiary ammonium ions for use as solvent in industrial and com. applications)

Amines, reactions

RL: RCT (Reactant); RACT (Reactant or reagent)

(primary; preparation and methods for manufacture of ionic liqs. containing protonated primary, secondary or tertiary ammonium ions)

Carboxylic acids, uses

Sulfonic acids, uses

RL: NUU (Other use, unclassified); USES (Uses)

(salts, anion component for ionic liquid; preparation and methods for nufacture

of ionic liqs. containing protonated primary, secondary or tertiary ammonium ions)

IT Amines, reactions

RL: RCT (Reactant); RACT (Reactant or reagent)

(secondary; preparation and methods for manufacture of ionic liqs. containing $% \left(1\right) =\left(1\right) +\left(1$

 $\,$ protonated primary, secondary or tertiary ammonium ions) $\,$ II $\,$ $\,$ Amines, reactions $\,$

RL: RCT (Reactant); RACT (Reactant or reagent)

(tertiary; preparation and methods for manufacture of ionic liqs. containing protonated primary, secondary or tertiary ammonium ions)

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56-14-4, Succinate, uses 57-60-3, Pyruvate, uses 63-36-5, Salicylate,
                  71-47-6, Formate, uses 71-50-1, Acetate, uses 71-52-3, Hydrogen
       carbonate, uses 72-03-7, Propanoate, uses 74-81-7, Octanoate, uses
       113-21-3, Lactate, uses 126-44-3, Citrate, uses 142-42-7, Fumarate,
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       338-70-5, uses 461-55-2, Butanoate, uses 666-14-8, uses 766-76-7,
       Benzoate, uses 769-61-9, Mandelate 3342-79-8, Nonanoate 3398-75-2,
       Decanoate 3715-17-1, Tartrate, uses 3812-32-6, Carbonate, uses
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                 14477-72-6, Trifluoroacetate ion, uses 14797-55-8, Nitrate, uses
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       Trifluoromethanesulfonate 41824-21-9, Crotonate 44864-55-3
       45048-62-2 49681-69-8, Hydrogen tartrate, uses
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       preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
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of ionic
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       20740-76-5
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       866567-33-1
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            ions)
       67-56-1, Methanol, reactions
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       50-00-0P, Formaldehyde, preparation
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- => s dimethylethanolammonium and formate
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- ANSWER 1 OF 2 CAPLUS COPYRIGHT 2009 ACS on STN
- AN 2008:165841 CAPLUS
- DN 148 - 238708
- Entered STN: 10 Feb 2008
- Solvent and Rotational Relaxation of Coumarin 153 in a Protic Ionic Liquid TΙ Dimethylethanolammonium Formate
- Seth, Debabrata; Sarkar, Souravi; Sarkar, Nilmoni AU
- CS Department of Chemistry, Indian Institute of Technology, Kharagpur, 721 302, India
- SO Journal of Physical Chemistry B (2008), 112(9), 2629-2636
- CODEN: JPCBFK; ISSN: 1520-6106
- PB American Chemical Society
- DT Journal
- LA English
- CC 22-9 (Physical Organic Chemistry)
- The solvent relaxation and orientational dynamics of coumarin 153 (C-153) was investigated in N,N-dimethylethanolammonium formate
- (DAF) with a variation of temperature DAF is a protic room-temperature ionic liquid,
 - comprised of nonarom. cations. Both solvent relaxation and orientational dynamics of C-153 in DAF are linearly well-correlated with the bulk viscosity at different temps. We optimized the geometry of DAF using quantum chemical calcns. using d. functional theory methods. The optimized structure of DAF shows a nonbonded interaction between cation and anion, which suggests that a hydrogen bond is formed between hydrogen atoms attached to the nitrogen atom of the cation with the oxygen atom of the anion in DAF.
- ST solvent rotational relaxation coumarin protic ionic lig dimethylethanolammonium formate
- Molecular structure TT
 - (optimized; solvent and rotational relaxation of coumarin 153 in protic ionic liquid dimethylethanolammonium formate)
 - Fluorescence
 - Hydrogen bond
 - Ionic liquids Molecular orientation

 - Molecular rotation Solvation
 - dimethylethanolammonium formate) 59101-30-3
- RL: NUU (Other use, unclassified); PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process); USES (Uses)
 - (solvent and rotational relaxation of coumarin 153 in protic ionic liquid dimethylethanolammonium formate)

(solvent and rotational relaxation of coumarin 153 in protic ionic liquid

- 53518-18-6, Coumarin 153
 - RL: PRP (Properties)
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dimethylethanolammonium formate)

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 - AN 2005:1090138 CAPLUS DN
 - 143:386681
 - Entered STN: 12 Oct 2005
 - Ionic liquids containing protonated primary, secondary or tertiary ammonium ions
 - IN Walker, Adam John
 - PA The University of York, UK
 - Brit. UK Pat. Appl., 62 pp. CODEN: BAXXDU
- Patent
- LA English
- IC ICM C07C215-08
 - ICS C07C215-12; C07C217-30
- 23-4 (Aliphatic Compounds)

Section cross-reference(s): 45

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	MX 200	73323 80115	31		A		2007	0326		MX 2	007-	1153	1		2	0061	
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					C07C												
			ECL	A	C07C	215/	40;	C07C	215/	08;	CU7C	215/	12;	CU7C	217/	30	

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CN 1997620
                TPCT
                       C07C0215-40 [I,A]; C07C0215-00 [I,C*]; B01J0031-04
                       [I,A]; B01J0031-02 [I,A]
                TPCR
                       C07C0215-00 [I,C]; C07C0215-40 [I,A]; C07C0215-08
                       [I,A]; C07C0215-12 [I,A]; C07C0217-00 [I,C*];
                       C07C0217-30 [I.A]
                ECLA
                       C07C215/40; C07C215/08; C07C215/12; C07C217/30
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EP 1805131
                IPCR
                       C07C0215-00 [I,C]; C07C0215-40 [I,A]; C07C0215-08
                       [I,A]; C07C0215-12 [I,A]; C07C0217-00 [I,C*];
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                       C07C215/40; C07C215/08; C07C215/12; C07C217/30
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                       [I,A]; C07C0311-00 [I,C*]
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                       C07C0217-30 [I,A]; C07C0311-00 [I,C]; C07C0311-03 [I,A]
                FTERM 4H006/AA01; 4H006/AA03; 4H006/AB80
MX 2006011531
                IPCI
                       B01J0031-02 [I,C*]; B01J0031-04 [I,C*]; C07C0215-40
                       [I,A]; C07C0215-00 [I,C*]
IN 2006KN03208
               IPCI
                       C07C0215-40 [ICM, 7]; C07C0215-00 [ICS, 7]
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                       C07C0215-40 [I,A]; C07C0215-00 [I,A]
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               IPCI
                       C07C0215-02 [I,A]; C07C0215-00 [I,C*]; C07D0211-02
                       [I,A]; C07D0211-00 [I,C*]
                NCL
                       546/184.000; 564/281.000
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OS MARPAT 143:386681

AB The present invention relates to ionic ligs. comprising an anion and a cation wherein the cation is a primary, secondary or tertiary ammonium ion containing a protonated nitrogen atom. The invention also provides processes for the manufacture of ionic ligs. For example, N,N-dimethylethanolammonium glycolate (I) was prepared by gradually adding glycolic acid to an alc. solution of N,N-dimethylethanolamine; after completion and neutralization, the cold alc. solution was filtered, solvent removed, then frozen in liquid nitrogen and lyophilized in vacuo. After gradually allowing the sample to warm to room temperature, 32.85 g (99% yield) of I as a pale yellow liquid was isolated. Preferred ionic ligs. contain ethanolammonium, diethanolammonium, N-butyldiethanolammonium, N,N-dimethylethanolammonium, N,N-methylethanolammonium, N,N-dimethylethanolammonium, N,N-methylethanolammonium,

N,N-di(methoxyethyl)ammonium and 1-(3-hydroxypropyl)putrescinium ions as cations.

amine acid; ammonium ionic liq prepn; primary ammonium ion prepn ionic

amine acid; ammonium ionic liq preph; primary ammonium ion preph ionic liq; secondary ammonium ion preph ionic liq; tertiary ammonium ion preph ionic liq

IT Oxidation

(enzymic; demonstration of application of ionic liqs. in enzymic oxidation of methanol to formaldehyde)

IT Green chemistry

Ionic liquids

(preparation and methods for manufacture of ionic liqs. containing protonated $% \left(1\right) =\left(1\right) \left(1\right) \left($

primary, secondary or tertiary ammonium ions)
IT Quaternary ammonium compounds, preparation

RL: IMF (Industrial manufacture); NUU (Other use, unclassified); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)

(preparation and methods for manufacture of ionic liqs. containing protonated

primary, secondary or tertiary ammonium ions)

IT Acids, reactions

RL: RCT (Reactant); RACT (Reactant or reagent) (preparation and methods for manufacture of ionic liqs. containing protonated

primary, secondary or tertiary ammonium ions)

IT Solvents

(preparation and methods for manufacture of ionic liqs. containing protonated $% \left(1\right) =\left(1\right) +\left(1$

primary, secondary or tertiary ammonium ions for use as solvent in industrial and com. applications)

I Amines, reactions

RL: RCT (Reactant); RACT (Reactant or reagent)

(primary; preparation and methods for manufacture of ionic liqs. containing protonated primary, secondary or tertiary ammonium ions)

T Carboxylic acids, uses Sulfonic acids, uses

RL: NUU (Other use, unclassified); USES (Uses)

(salts, anion component for ionic liquid; preparation and methods for

manufacture
 of ionic liqs. containing protonated primary, secondary or tertiary
 ammonium ions)

Amines, reactions

RL: RCT (Reactant); RACT (Reactant or reagent)

(secondary; preparation and methods for manufacture of ionic liqs. containing $% \left(1\right) =\left(1\right) +\left(1$

protonated primary, secondary or tertiary ammonium ions)

IT Amines, reactions

866621-22-9

RL: RCT (Reactant); RACT (Reactant or reagent)

(tertiary; preparation and methods for manufacture of ionic liqs. containing protonated primary, secondary or tertiary ammonium ions)

56-14-4, Succinate, uses 57-60-3, Pyruvate, uses 63-36-5, Salicylate, 71-47-6, Formate, uses 71-50-1, Acetate, uses 71-52-3, Hydrogen carbonate, uses 72-03-7, Propanoate, uses 74-81-7, Octanoate, uses 113-21-3, Lactate, uses 126-44-3, Citrate, uses 142-42-7, Fumarate, uses 149-61-1, Malate 150-43-6, uses 151-33-7, Hexanoate, uses 338-70-5, uses 461-55-2, Butanoate, uses 666-14-8. uses 766-76-7, Benzoate, uses 769-61-9, Mandelate 3342-79-8, Nonanoate 3398-75-2, Decanoate 3715-17-1, Tartrate, uses 3812-32-6, Carbonate, uses 7563-37-3, Heptanoate 7631-42-7, Phenylacetate, uses 10023-74-2, Pentanoate, uses 12627-13-3, Silicate 14066-19-4, Hydrogen phosphate, uses 14066-20-7, Dihydrogen phosphate, uses 14265-44-2, Phosphate, uses 14477-72-6, Trifluoroacetate ion, uses 14797-55-8, Nitrate, uses 14808-79-8, Sulphate, uses 14874-70-5, Tetrafluoroborate 14996-02-2, Hydrogen sulfate, uses 16053-58-0, Methanesulfonate anion 16887-00-6, Chloride, uses 16919-18-9, Hexafluorophosphate Metaphosphate (P40124-) 20461-54-5, Iodide, uses Pantothenate 24959-67-9, Bromide, uses 37181-39-8, Trifluoromethanesulfonate 41824-21-9, Crotonate 44864-55-3

Trifluoromethanesulfonate 41824-21-9, Crotonate 44864-55-3 45048-62-2 49681-69-8, Hydrogen tartrate, uses 59561-61-4 86848-98-8 86848-99-9 97901-86-5 98837-98-0 130434-58-1 328238-56-8

RL: NUU (Other use, unclassified); USES (Uses)

(anion component for ionic liquid; preparation and methods for manufacture of ionic liqs. containing protonated primary, secondary or tertiary ammonium ions)

176158-74-0P

RL: BSU (Biological study, unclassified); IMF (Industrial manufacture); NUU (Other use, unclassified); PRP (Properties); SPN (Synthetic

preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)

(biodegrdn. anal. of ionic liquid; preparation and methods for manufacture of ionic

ligs. containing protonated primary, secondary or tertiary ammonium ions) 17 20740-76-5 22892-66-0, Ethanolamine conjugate acid 26265-71-4 36833-63-3 36833-64-4 65591-62-0 90578-97-5 866567-32-0 866567-33-1 866567-34-2

RL: NUU (Other use, unclassified); USES (Uses)

(cation component for ionic liquid; preparation and methods for manufacture

ionic liqs. containing protonated primary, secondary or tertiary ammonium ions)

IT 67-56-1, Methanol, reactions

RL: RCT (Reactant); RACT (Reactant or reagent)

(demonstration of application of ionic liqs. in enzymic oxidation of methanol to formaldehyde)

IT 50-00-0P, Formaldehyde, preparation

RL: SPN (Synthetic preparation); PREP (Preparation)

(demonstration of application of ionic liqs. in enzymic oxidation of methanol to formaldehyde)

2471-06-9P 2604-13-9P 2805-17-6P 3178-20-9P 4337-66-0P 5988-51-2P 7487-79-8P 16530-72-6P 16830-40-3P 17618-31-4P 17618-32-5P 17863-38-6P 18394-23-5P 20261-59-0P 20475-13-2P 20748-72-5P 21829-52-7P 23251-72-1P, Diethanolamine acetate 23349-61-3P 25859-29-4P 26764-31-8P 28098-03-5P 28129-21-7P. Diethanolamine hydrobromide 29194-47-6P 29867-71-8P 29867-72-9P 29867-75-2P 29868-00-6P 29868-01-7P 29870-14-2P 29870-15-3P 29870-25-5P 29870-26-6P 29870-18-6P 29870-19-7P 29870-27-7P 30933-06-3P 31086-83-6P 31889-13-1P 29870-29-9P 30718-92-4P 35423-90-6P 38491-11-1P 38739-74-1P 49753-18-6P 49753-20-0P 51264-32-5P 51276-44-9P 53226-35-0P 53562-95-1P 53926-87-7P 54300-24-2P 55756-39-3P 56409-18-8P 56669-87-5P 57117-29-0P 58937-21-6P 59101-30-3P 59866-70-5P 60395-28-0P 62036-98-0P 63517-71-5P 63517-72-6P 64601-03-2P 64601-04-3P 64601-14-5P 67303-52-0P 67384-57-0P 68141-00-4P 68141-46-8P 68391-54-8P. Diethanolamine formate 68568-51-4P 68815-69-0P 68833-69-2P 68860-57-1P 68945-90-4P 69362-00-1P 69362-01-2P 75478-96-5P 76788-90-4P 77534-73-7P 79266-74-3P 82801-62-5P 77534-69-1P 84110-42-9P 84145-30-2P 84145-60-8P 84176-56-7P 86683-38-7P 86683-39-8P 88331-27-5P 89855-93-6P 90000-02-5P 90434-46-1P 93882-26-9P 93882-27-0P 93942-28-0P 93942-29-1P 95332-67-5P 98005-86-8P 98837-33-3P 101901-23-9P 103079-19-2P 108067-35-2P 109962-24-5P 111318-69-5P 116033-27-3P 117472-14-7P 126050-30-4P 134227-25-1P 135691-53-1P 137360-57-7P 138036-64-3P 156814-01-6P 164460-12-2P 181180-62-1P 205490-53-5P 205490-69-3P 209052-82-4P 210040-56-5P 252280-99-2P 327156-58-1P 372169-26-1P 372169-30-7P 392292-52-3P 815574-85-7P 857086-60-3P 857086-63-6P 866567-31-9P 866567-31-9P 866567-35-3P 866567-36-4P 866567-37-5P 866567-38-6P 866567-39-7P 866567-40-0P 866567-41-1P 866567-42-2P 866567-43-3P 866567-44-4P 866567-45-5P 866567-46-6P 866567-47-7P 866567-48-8P 866567-49-9P 866567-50-2P 866567-51-3P 866567-52-4P 866567-53-5P 866567-54-6P 866567-55-7P 866567-56-8P 866567-57-9P 866567-58-0P 866567-59-1P 866567-60-4P 866567-61-5P 866567-62-6P 866567-63-7P 866567-65-9P 866567-67-1P 866567-69-3P 866567-70-6P 866567-71-7P 866567-72-8P 866567-73-9P 866567-74-0P 866567-75-1P 866567-76-2P 866567-77-3P 866567-78-4P 866567-79-5P 866567-80-8P 866567-81-9P 866567-82-0P 866567-83-1P 866567-84-2P 866567-85-3P 866567-86-4P 866567-87-5P 866567-88-6P 866567-89-7P 866567-90-0P 866567-91-1P 866567-92-2P 866567-93-3P 866567-94-4P 866567-95-5P 866567-96-6P 866567-97-7P 866567-98-8P 866567-99-9P 866568-00-5P 866568-01-6P 866568-02-7P 866568-03-8P 866568-04-9P 866568-05-0P 866568-06-1P 866568-07-2P 866568-08-3P 866568-09-4P 866568-10-7P 866568-11-8P 866568-13-0P 866568-15-2P 866568-16-3P 866568-12-9P 866568-17-4P 866568-19-6P 866568-21-0P 866568-20-9P 866568-22-1P 866568-18-5P 866568-26-5P 866568-23-2P 866568-24-3P 866568-25-4P 866568-27-6P 866568-31-2P 866568-32-3P 866568-28-7P 866568-29-8P 866568-30-1P 866568-33-4P 866568-34-5P 866568-35-6P 866568-36-7P 866568-37-8P 866568-38-9P 866568-39-0P 866568-40-3P 866568-41-4P 866568-42-5P 866568-43-6P

RL: IMF (Industrial manufacture); NUU (Other use, unclassified); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)

(preparation and methods for manufacture of ionic liqs. containing protonated

	secondary or tert			
866568-44-7P	866568-45-8P	866568-46-9P	866568-47-0P	866568-48-1P
866568-49-2P	866568-50-5P	866568-51-6P	866568-52-7P	866568-53-8P
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866568-69-6P	866568-70-9P	866568-71-0P	866568-72-1P	866568-74-3P
866568-75-4P	866568-76-5P	866568-78-7P	866568-79-8P	866568-80 - 1P
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866569-86-0P	866569-87-1P	866569-88-2P	866569-89-3P	866569-90-6P
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(Synthetic preparation); PREP (Preparation); USES (Uses) (preparation and methods for manufacture of ionic ligs. containing protonated

primary, secondary or tertiary ammonium ions) 866571-03-1P 866571-04-2P 866570-97-0P 866570-99-2P 866571-01-9P 866571-05-3P 866571-06-4P 866571-07-5P 866571-08-6P 866571-09-7P 866571-10-0P 866571-11-1P 866571-12-2P 866571-13-3P 866571-14-4P 866571-15-5P 866571-16-6P 866571-17-7P 866571-18-8P 866571-19-9P 866571-20-2P 866571-22-4P 866571-23-5P 866571-21-3P 866571-24-6P 866571-25-7P 866571-26-8P 866571-27-9P 866571-28-0P 866571-29-1P 866571-30-4P 866571-31-5P 866571-32-6P 866571-33-7P 866571-34-8P 866571-35-9P 866571-36-0P 866571-37-1P 866571-38-2P 866571-39-3P 866571-44-0P 866571-40-6P 866571-41-7P 866571-42-8P 866571-43-9P

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(preparation and methods for manufacture of ionic liqs. containing protonated

primary, secondary or tertiary ammonium ions)

IT 79-14-1, Glycolic acid, reactions 102-79-4, N-Butyldiethanolamine 108-01-0, N,N-Dimethylethanolamine 82113-65-3

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation and methods for manufacture of ionic liqs. containing protonated

primary, secondary or tertiary ammonium ions)
RE.CNT 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD

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- => s 59101-30-3/rn or 53518-18-6/rn
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 - 2 59101-30-3/RN OR 53518-18-6/RN

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- 4 ANSWER 1 OF 2 REGISTRY COPYRIGHT 2009 ACS on STN
- RN 59101-30-3 REGISTRY
- ED Entered STN: 16 Nov 1984
- CN Formic acid, compd. with 2-(dimethylamino)ethanol (1:1) (CA INDEX NAME) OTHER CA INDEX NAMES:
- CN Ethanol, 2-(dimethylamino)-, formate (salt) (9CI)
- OTHER NAMES:
- CN 2-(Dimethylamino)ethanol formate (salt)
- CN Dimethylethanolamine formate
- MF C4 H11 N O . C H2 O2
- C STN Files: CA, CAPLUS, CHEMLIST, TOXCENTER, USPATFULL

Other Sources: EINECS**, NDSL**, TSCA**

(**Enter CHEMLIST File for up-to-date regulatory information)

CRN 108-01-0 CMF C4 H11 N O Me2N-CH2-CH2-OH CM 2 CRN 64-18-6 CMF C H2 O2 о== сн- он 6 REFERENCES IN FILE CA (1907 TO DATE) 1 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA 6 REFERENCES IN FILE CAPLUS (1907 TO DATE) ANSWER 2 OF 2 REGISTRY COPYRIGHT 2009 ACS on STN 53518-18-6 REGISTRY Entered STN: 16 Nov 1984 1H, 5H, 11H-[1]Benzopyrano[6,7,8-ij]quinolizin-11-one, 2,3,6,7-tetrahydro-9-(trifluoromethyl)- (CA INDEX NAME) OTHER NAMES: C 153 C 6F Coumarin 153 Coumarin 495 Coumarin 540A Coumarin 6F K 153 NSC 338964 Pilot 495 59977-81-0 C16 H14 F3 N O2 COM STN Files: BEILSTEIN*, BIOSIS, CA, CAPLUS, CASREACT, CHEMCATS, CHEMLIST,

(*File contains numerically searchable property data) Other Sources: EINECS**, NDSL**, TSCA** (**Enter CHEMLIST File for up-to-date regulatory information)

CSCHEM, DDFU, DRUGU, IFICDB, IFIPAT, IFIUDB, MSDS-OHS, TOXCENTER,

USPAT2, USPATFULL

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569 REFERENCES IN FILE CAPLUS (1907 TO DATE)

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=> s 59101-30-3 REG1stRY INITIATED

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L6 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2009 ACS on STN AN 2008:165841 CAPLUS

- DN 148:238708
- Entered STN: 10 Feb 2008
- Solvent and Rotational Relaxation of Coumarin 153 in a Protic Ionic Liquid Dimethylethanolammonium Formate
- AΠ Seth, Debabrata; Sarkar, Souravi; Sarkar, Nilmoni
- CS Department of Chemistry, Indian Institute of Technology, Kharagpur, 721 302, India
- SO Journal of Physical Chemistry B (2008), 112(9), 2629-2636
- CODEN: JPCBFK; ISSN: 1520-6106
- PR American Chemical Society
- DT Journal
- LA English
- CC 22-9 (Physical Organic Chemistry)
- AB The solvent relaxation and orientational dynamics of coumarin 153 (C-153) was investigated in N,N-dimethylethanolammonium formate (DAF) with a variation of temperature DAF is a protic room-temperature ionic liquid,

comprised of

nonarom. cations. Both solvent relaxation and orientational dynamics of C-153 in DAF are linearly well-correlated with the bulk viscosity at different temps. We optimized the geometry of DAF using quantum chemical calcns. using d. functional theory methods. The optimized structure of DAF shows a nonbonded interaction between cation and anion, which suggests that a hydrogen bond is formed between hydrogen atoms attached to the nitrogen atom of the cation with the oxygen atom of the anion in DAF.

- solvent rotational relaxation coumarin protic ionic liq dimethylethanolammonium formate
- Molecular structure

(optimized; solvent and rotational relaxation of coumarin 153 in protic ionic liquid dimethylethanolammonium formate)

- Fluorescence
 - Hydrogen bond
 - Ionic liquids Molecular orientation
 - Molecular rotation
 - Solvation

(solvent and rotational relaxation of coumarin 153 in protic ionic liquid dimethylethanolammonium formate)

- 59101-30-3
 - RL: NUU (Other use, unclassified); PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process); USES (Uses)
 - (solvent and rotational relaxation of coumarin 153 in protic ionic liquid dimethylethanolammonium formate)
 - 53518-18-6, Coumarin 153
 - RL: PRP (Properties)

(solvent and rotational relaxation of coumarin 153 in protic ionic liquid dimethylethanolammonium formate) RE.CNT 105 THERE ARE 105 CITED REFERENCES AVAILABLE FOR THIS RECORD

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    Entered STN: 15 Jun 2006
TI
    Additive and vehicle for aqueous inks, paints, coatings and adhesives
TN
    Skov, Richard T.; Cook, Leroy John
PA
    Omnitech Environmental, LLC, USA
SO
     PCT Int. Appl., 55 pp.
     CODEN: PIXXD2
DT
     Patent
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     42-10 (Coatings, Inks, and Related Products)
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CLASS
 PATENT NO.
                CLASS PATENT FAMILY CLASSIFICATION CODES
                IPCI
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 WO 2006063266
                        [I,A]; C09D0133-00 [I,C]; C09D0133-00 [I,A]
                 IPCR
                       C09D0133-00 [I,C]; C09D0133-00 [I,A]
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US 20060128831
                IPCI
                       C03C0017-00 [I,A]; C09D0011-00 [I,A]
                 NCL
                       523/160.000; 523/161.000
                 ECLA
                       C09J133/04
    Additives for improving the film formation of inks, paints, coatings, and
     adhesives are based on photocurable products of carboxylic acids or
     anhydrides with N-alkylalkanolamines or dialkylaminoalkyl (meth)acrylates.
     A typical additive was manufactured by slowly adding 1.75 lbs
     dimethylaminoethyl methacrylate to 2.5 lbs water containing 1 lb
     4,4'-carbonylbis(1,2-benzenedicarboxylic acid).
     film promoter photocurable carboxylate dialkylaminoalkyl methacrylate ink
     paint adhesive; carbonylbisphthalic acid dimethylaminoethyl methacrylate
     salt manuf
     Paints
        (latex; photocurable carboxylic acid salts of amines as additives for
        improving film formation of inks, paints, coatings and adhesives)
     Inks
        (oil-based; photocurable carboxylic acid salts of amines as additives
        for improving film formation of inks, paints, coatings and adhesives)
     Quaternary ammonium compounds, uses
     RL: IMF (Industrial manufacture); MOA (Modifier or additive use); TEM
     (Technical or engineered material use); PREP (Preparation); USES (Uses)
        (photocurable carboxylic acid salts of amines as additives for
        improving film formation of inks, paints, coatings and adhesives)
     Acrylic polymers, uses
     Polyurethanes, uses
     RL: POF (Polymer in formulation); TEM (Technical or engineered material
     use); USES (Uses)
        (photocurable carboxylic acid salts of amines as additives for
        improving film formation of inks, paints, coatings and adhesives)
     Carboxylic acids, uses
     RL: IMF (Industrial manufacture); MOA (Modifier or additive use); TEM
     (Technical or engineered material use); PREP (Preparation); USES (Uses)
        (salts; photocurable carboxylic acid salts of amines as additives for
        improving film formation of inks, paints, coatings and adhesives)
     Corn oil
     Cottonseed oil
     Linseed oil
     Olive oil
     Palm kernel oil
     Palm oil
     Peanut oil
     Sovbean oil
     Tall oil
     Tung oil
     RL: TEM (Technical or engineered material use); USES (Uses)
        (vehicle; photocurable carboxylic acid salts of amines as additives for
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improving film formation of inks, paints, coatings and adhesives) Adhesives

Coating materials

(water-thinned; photocurable carboxylic acid salts of amines as additives for improving film formation of inks, paints, coatings and adhesives)

890650-25-6, PS 68

RL: POF (Polymer in formulation); TEM (Technical or engineered material

use); USES (Uses)

(adhesive; photocurable carboxylic acid salts of amines as additives for improving film formation of inks, paints, coatings and adhesives) 890309-29-2P 890650-27-8P

RL: IMF (Industrial manufacture): TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)

(cured coating; photocurable carboxylic acid salts of amines as additives for improving film formation of inks, paints, coatings and adhesives)

50-21-5DP, Lactic acid, salts with amines 50-78-2DP, Acetylsalicylic acid, salts with amines 57-10-3DP, Palmitic acid, salts with amines 57-11-4DP, Stearic acid, salts with amines 64-18-6DP, Formic acid, salts with amines 64-19-7DP, Acetic acid, salts with amines 65-85-0DP, Benzoic acid, salts with amines 77-92-9DP, Citric acid, salts with amines 79-09-4DP, Propionic acid, salts with amines 79-10-7DP, Acrylic acid, salts with amines 79-11-8DP, Chloroacetic acid, salts with amines 79-14-1DP, Glycolic acid, salts with amines 79-41-4DP, Methacrylic acid, salts with amines 85-52-9DP, o-Benzoylbenzoic acid, salts with amines 87-69-4DP, Tartaric acid, salts with amines 88-99-3DP, Phthalic acid, salts with amines 97-65-4DP, Itaconic acid, salts with amines 99-50-3DP, Protocatechuic acid, salts with amines 100-21-0DP, Terephthalic acid, salts with amines 100-37-8DP, N.N-Diethylethanolamine, salts with carboxylic acids 105-16-8DP, N, N-Diethylaminoethyl methacrylate, salts with carboxylic acids 105-59-9DP, N-Methyldiethanolamine, salts with carboxylic acids 108-01-0DP, N,N-Dimethylethanolamine, salts with carboxylic acids 108-30-5DP, Succinic anhydride, salts with amines 108-31-6DP, Maleic anhydride, salts with amines 108-55-4DP, Glutaric anhydride, salts with 109-83-1DP, N-Methylethanolamine, salts with carboxylic acids 110-15-6DP, Succinic acid, salts with amines 110-16-7DP, Maleic acid, salts with amines 110-17-8DP, Fumaric acid, salts with amines 111-20-6DP, Sebacic acid, salts with amines 112-80-1DP, Oleic acid, salts with amines 121-91-5DP, Isophthalic acid, salts with amines 124-04-9DP, Adipic acid, salts with amines 141-22-0DP, Ricinoleic acid, salts with amines 141-82-2DP, Malonic acid, salts with amines 144-62-7DP, Oxalic acid, salts with amines 485-38-1DP, 4,5-Dimethoxyisophthalic acid, salts with amines 514-10-3DP, Abietic acid, salts with amines 526-95-4DP, D-Gluconic acid, salts with amines 1585-40-6DP, Benzenepentacarboxylic acid, salts with amines Benzophenonetetracarboxylic acid dianhydride, salts with amines 2426-54-2DP, N.N-Diethylaminoethyl acrylate, salts with carboxylic acids 2439-35-2DP, salts with carboxylic acids 2479-49-4DP, 3,3',4,4'-Benzophenonetetracarboxylic acid, salts with amines 2867-47-2DP, N,N-Dimethylaminoethyl methacrylate, salts with carboxylic acids 2893-43-8DP, N-Ethyl-N-methylethanolamine, salts with carboxylic acids 5570-18-3DP, 2-Aminobenzeneboronic acid, salts with amines 6660-65-7DP, 4,6-Dichloroisophthalic acid, salts with amines 6939-93-1DP, 4-Bromoisophthalic acid, salts with amines 13049-16-6DP, salts with amines 21161-11-5DP, 2-Nitroisophthalic acid, salts with amines 30755-77-2DP, Benzophenonedicarboxylic acid, salts with amines 39622-79-2DP, 2-Aminoisophthalic acid, salts with amines 52125-39-0DP, salts with carboxylic acids 59101-30-3P 60047-46-3DP, salts with amines 116631-90-4DP, salts with amines 255731-44-3DP, salts with carboxylic acids 890309-27-0P 890309-28-IP 890639-88-DP, salts with carboxylic acids 890639-92-6DP, salts with carboxylic acids RL: IMF (Industrial manufacture); MOA (Modifier or additive use); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses) (photocurable carboxylic acid salts of amines as additives for

improving film formation of inks, paints, coatings and adhesives) 890650-05-2, Filtrez 5014 RL: POF (Polymer in formulation); TEM (Technical or engineered material

200359-24-6, Carboset GA 1931 223784-68-7, Maincote HG 54D

use); USES (Uses)

(photocurable carboxylic acid salts of amines as additives for improving film formation of inks, paints, coatings and adhesives)

THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD RE.CNT 1 RE

- (1) Anon; WO 2004044067 A1 CAPLUS
- L6 ANSWER 3 OF 6 CAPLUS COPYRIGHT 2009 ACS on STN
- AN 2005:1090138 CAPLUS
- DN 143:386681
- ED Entered STN: 12 Oct 2005
- TΙ Ionic liquids containing protonated primary, secondary or tertiary ammonium ions
- TN Walker, Adam John
- PA The University of York, UK
- Brit. UK Pat. Appl., 62 pp. SO CODEN: BAXXDU
- DT Patent
- LA English
- ΙĊ ICM C07C215-08
- ICS C07C215-12; C07C217-30
- CC 23-4 (Aliphatic Compounds) Section cross-reference(s): 45

GB 2412912

TCM

TCS

C07C215-08

C07C215-12; C07C217-30

C07C0215-00 [I,C]; C07C0215-08 [I,A]; C07C0215-12 [I,A]; C07C0217-00 [I,C]; C07C0217-30 [I,A]

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ΡI	GB	2412 2412 2005 2563 2005	912			A		2005	1012		GB	20	05-	6984			2	0050	407
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	WO	2005	0977.	31		A3		2005	1124										
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		R:						CZ,										HU,	ΙE,
								MC,											
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	IN	2006	KN03:	208		A		2007	0608		ΙN	20	06-1	KN32	80		2	0061	103
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	US	2007	0185	330		A1		2007	0809		US	20	07-	5996	94		2	0070	119
PRAI	GB	2004 2005	-790	8		A		2004	0407										
	WO	2005	-GB1	364		W		2005	0407										
CLAS PAT		NO.		CLA	ss	PATE	NT F	AMTL	y CL	ASST	FIC	דמי	TON	COD	ES				

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TPCR
                      C07C0215-00 [I,C]; C07C0215-08 [I,A]; C07C0215-12
                       [I,A]; C07C0215-40 [I,A]; C07C0217-00 [I,C];
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AU 2005232025
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                ECLA
                       C07C215/40; C07C215/08; C07C215/12; C07C217/30
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                       B01J0031-04 [I,A]; C07C0215-08 [I,A]; C07C0215-12
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WO 2005097731
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                       C07C215/40; C07C215/08; C07C215/12; C07C217/30
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                FTERM 4H006/AA01; 4H006/AA03; 4H006/AB80
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                       [I,A]; C07C0215-00 [I,C*]
IN 2006KN03208 IPCI
                       C07C0215-40 [ICM, 7]; C07C0215-00 [ICS, 7]
KR 2007031302 IPCI
                       C07C0215-40 [I.A]; C07C0215-00 [I.A]
US 20070185330 IPCI
                       C07C0215-02 [I,A]; C07C0215-00 [I,C*]; C07D0211-02
                       [I,A]; C07D0211-00 [I,C*]
                NCL.
                       546/184.000; 564/281.000
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OS MARPAT 143:386681

ST amine acid; ammonium ionic liq prepn; primary ammonium ion prepn ionic liq; secondary ammonium ion prepn ionic liq; tertiary ammonium ion prepn

AB The present invention relates to ionic ligs, comprising an anion and a cation wherein the cation is a primary, secondary or tertiary ammonium ion containing a protonated nitrogen atom. The invention also provides processes for the manufacture of ionic ligs. For example, N,N-dimethylethanolammonium glycolate (I) was prepared by gradually adding glycolic acid to an alc. solution of N,N-dimethylethanolamine; after completion and neutralization, the cold alc. solution was filtered, solvent removed, then frozen in liquid nitrogen and lyophilized in vacuo. After gradually allowing the sample to warm to room temperature, 32.85 g (99% yield) of I as a pale yellow liquid was isolated. Preferred ionic liqs. contain ethanolammonium, diethanolammonium, N-butyldiethanolammonium, N,N-dimethylethanolammonium, N-methylethanolammonium, N, N-di(methoxyethyl)ammonium and 1-(3-hydroxypropyl)putrescinium ions as cations.

ionic lig Oxidation (enzymic; demonstration of application of ionic ligs. in enzymic oxidation of methanol to formaldehyde) Green chemistry Ionic liquids (preparation and methods for manufacture of ionic ligs. containing protonated primary, secondary or tertiary ammonium ions) Quaternary ammonium compounds, preparation RL: IMF (Industrial manufacture); NUU (Other use, unclassified); SPN (Synthetic preparation); PREP (Preparation); USES (Uses) (preparation and methods for manufacture of ionic ligs. containing protonated primary, secondary or tertiary ammonium ions) Acids, reactions RL: RCT (Reactant); RACT (Reactant or reagent) (preparation and methods for manufacture of ionic liqs. containing protonated primary, secondary or tertiary ammonium ions) Solvents (preparation and methods for manufacture of ionic ligs, containing protonated primary, secondary or tertiary ammonium ions for use as solvent in industrial and com. applications) Amines, reactions RL: RCT (Reactant); RACT (Reactant or reagent) (primary; preparation and methods for manufacture of ionic ligs. containing protonated primary, secondary or tertiary ammonium ions) Carboxylic acids, uses Sulfonic acids, uses RL: NUU (Other use, unclassified); USES (Uses) (salts, anion component for ionic liquid; preparation and methods for manufacture of ionic liqs. containing protonated primary, secondary or tertiary ammonium ions) Amines, reactions RL: RCT (Reactant); RACT (Reactant or reagent) (secondary; preparation and methods for manufacture of ionic ligs. containing protonated primary, secondary or tertiary ammonium ions) Amines, reactions RL: RCT (Reactant); RACT (Reactant or reagent) (tertiary; preparation and methods for manufacture of ionic ligs. containing protonated primary, secondary or tertiary ammonium ions) 56-14-4, Succinate, uses 57-60-3, Pyruvate, uses 63-36-5, Salicylate, 71-50-1, Acetate, uses 71-47-6, Formate, uses 71-52-3, Hydrogen carbonate, uses 72-03-7, Propanoate, uses 74-81-7, Octanoate, uses 113-21-3, Lactate, uses 126-44-3, Citrate, uses 142-42-7, Fumarate, 149-61-1, Malate 150-43-6, uses 151-33-7, Hexanoate, uses 461-55-2, Butanoate, uses 666-14-8, uses 338-70-5, uses 766-76-7, 769-61-9, Mandelate 3342-79-8, Nonanoate 3398-75-2, Benzoate, uses Decanoate 3715-17-1, Tartrate, uses 3812-32-6, Carbonate, uses 7563-37-3, Heptanoate 7631-42-7, Phenylacetate, uses 10023-74-2, Pentanoate, uses 12627-13-3, Silicate 14066-19-4, Hydrogen phosphate, 14066-20-7, Dihydrogen phosphate, uses 14265-44-2, Phosphate, uses 14477-72-6, Trifluoroacetate ion, uses 14797-55-8, Nitrate, uses 14808-79-8, Sulphate, uses 14874-70-5, Tetrafluoroborate 14996-02-2, Hydrogen sulfate, uses 16053-58-0, Methanesulfonate anion

Chloride, uses 16919-18-9, Hexafluorophosphate 17121-12-9, Metaphosphate (P40124-) 20461-54-5, Iodide, uses 20938-62-9, Pantothenate 24959-67-9, Bromide, uses 37181-39-8,

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Trifluoromethanesulfonate
                                                 41824-21-9, Crotonate 44864-55-3
                           49681-69-8, Hydrogen tartrate, uses 59561-61-4
       45048-62-2
                                                                                                           86848-98-8
                           97901-86-5 98837-98-0 130434-58-1 328238-56-8
       86848-99-9
       866621-22-9
       RL: NUU (Other use, unclassified); USES (Uses)
            (anion component for ionic liquid; preparation and methods for manufacture
of ionic
            ligs. containing protonated primary, secondary or tertiary ammonium ions)
       176158-74-0P
       RL: BSU (Biological study, unclassified); IMF (Industrial manufacture);
       NUU (Other use, unclassified); PRP (Properties); SPN (Synthetic
       preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
            (biodegrdn. anal. of ionic liquid; preparation and methods for manufacture
of ionic
            liqs. containing protonated primary, secondary or tertiary ammonium ions)
       20740-76-5 22852-66-0, Ethanolamine conjugate acid 26265-71-4
                           36833-64-4 65591-62-0 90578-97-5 866567-32-0
       36833-63-3
       866567-33-1
                           866567-34-2
       RL: NUU (Other use, unclassified); USES (Uses)
            (cation component for ionic liquid; preparation and methods for manufacture
            ionic ligs, containing protonated primary, secondary or tertiary ammonium
            ions)
       67-56-1, Methanol, reactions
       RL: RCT (Reactant); RACT (Reactant or reagent)
            (demonstration of application of ionic ligs, in enzymic oxidation of
            methanol to formaldehyde)
       50-00-0P, Formaldehyde, preparation
       RL: SPN (Synthetic preparation); PREP (Preparation)
            (demonstration of application of ionic ligs. in enzymic oxidation of
            methanol to formaldehyde)
                                                                  3178-20-9P
       2471-06-9P 2604-13-9P
                                              2805-17-6P
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                                                                     16830-40-3P
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                                                                                             20475-13-2P
       20748-72-5P 21829-52-7P 23251-72-1P, Diethanolamine acetate
       23349-61-3P 25859-29-4P 26764-31-8P 28098-03-5P 28129-21-7P.
       Diethanolamine hydrobromide 29194-47-6P 29867-71-8P 29867-72-9P
       29867-75-2P 29868-00-6P 29868-01-7P 29870-14-2P 29870-15-3P
       29870-18-6P 29870-19-7P
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       29870-29-9P 30718-92-4P 30933-06-3P 31086-83-6P 31889-13-1P
       35423-90-6P 38491-11-1P 38739-74-1P 49753-18-6P 49753-20-0P
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       54300-24-2P 55756-39-3P 56409-18-8P 56669-87-5P 57117-29-0P
       58937-21-6P 59101-30-3P 59866-70-5P 60395-28-0P
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       64601-14-5P 67303-52-0P
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       68391-54-8P, Diethanolamine formate 68568-51-4P 68815-69-0P
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     79-14-1, Glycolic acid, reactions 102-79-4, N-Butyldiethanolamine
     108-01-0, N, N-Dimethylethanolamine 82113-65-3
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RE.CNT 7
             THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD
(1) Arizona State Univ; WO 2004114445 A1 CAPLUS
(2) Armstrong, D; Anal Chem 2001, V73, P3679 CAPLUS
(3) Basf; WO 2004090066 A1 CAPLUS
(4) Solvent Innovation; WO 03074494 A1 CAPLUS
(5) Staatliches Institut; DD 262042 A1 CAPLUS
(6) Studiengesellschaft; WO 03060057 A1 CAPLUS
(7) Williams, E; The J of Physical Chem 1977, V81(3) CAPLUS
     ANSWER 4 OF 6 CAPLUS COPYRIGHT 2009 ACS on STN
     1981:31600 CAPLUS
     94:31600
OREF 94:5217a,5220a
    Entered STN: 12 May 1984
    Stabilization of amine catalysts in a composition with halogenated polyols
     for polyurethane foam production
    Fuzesi, Stephen
PA Olin Corp., USA
SO U.S., 6 pp. Cont.-in-part of U.S. Ser. No. 801,676, abandoned.
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CODEN: USXXAM

DT Patent LA English IC C08G041-00 INCL 521171000

CC 36-6 (Plastics Manufacture and Processing)

FAN.CNT 2 PATENT NO. KIND DATE APPLICATION NO. DATE

PATENT NO.

PI US 4219624 GB 1586019 BR 7803348 JP 5314929 JP 6104192 FR 2393024 FR 2393024 PRAI US 1977-80 CLASS PATENT NO.	9	A 19800826 US 1978-962537 19781120 A 19810311 GB 1978-16548 19780426 A 19790116 BR 1978-3348 19780526 A 19781226 JP 1978-64854 19780530 B 19860918 A1 19781229 FR 1978-16143 19780530 B1 19820625 A2 19770531 PATENT FAMILY CLASSIFICATION CODES
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US 4219624	IC INCL IPCI IPCR	C08G041-00 521171000 C08G0041-00 [ICM] C08G0018-00 [I,C*]; C08G0018-18 [I,A]; C08G0018-50 [I,A] 521/171.000; 252/181.000; 521/112.000; 521/114.000;
		521/116.000; 521/131.000
	ECLA	C08G018/18R; C08G018/50C3
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	ECLA	C08G018/18R; C08G018/50C3; C08G065/26C1
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FR 2393024	IPCI	C08L0071-00 [ICM]; C08G0018-14 [ICS]; C08K0005-17 [ICS]; C08K0005-00 [ICS,C*]
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AB Storage-stable compns. for polyurethane foam manufacture contain a halogenated polyether polyol and .apprx.0.02-5% acid-blocked amine polyurethane foaming catalyst prepared by reacting a carboxylic acid with a tertiary amine at a molar ratio of .apprx.1-1.5:1. Thus, a series of amine-catalyzed, halogenated polyol compns., prepared by adding blocked, i.e., triethylenediamine diformate [40741-91-1], and unblocked, i.e., dimethylethanolamine, amine catalysts to a chlorinated polyether polyol (I) (OH number .apprx.365) prepared from 4,4,4-trichloro-1,2-epoxybutane and an equimolar ethylene glycol- α -D-glucose monohydrate mixture in the presence of BF3 etherate, were tested for pH, C1-, and available N+ before and after aging for 90 h at 60°. The results indicated prereaction with the halogenated polyol was minimized by acid blocking the amine

catalyst to prevent deactivation and loss of catalyst reactivity in a foaming reaction.

ST chlorinated polyol storage stability; polyurethane foam catalyst

stabilization; amine catalyst acid blocked

Polyoxyalkylenes RL: USES (Uses)

RL: USES (Uses)

(acid-blocked amine catalysts for, storage-stable)

IT Polymerization catalysts

(amines, acid-blocked, for halogenated polyols for polyurethane foam manufacture)

IT Urethane polymers, preparation

RL: PREP (Preparation)

(cellular, chlorinated polyether polyols for manufacture of, acid-blocked storage-stable amine catalysts for)

IT 502-44-3D, chlorinated polyol derivs. 629-11-8D, chlorinated polyol

derivs. 58450-04-7 76125-67-2

RL: USES (Uses)

(acid-blocked amine catalysts for, storage-stable)

IT 40741-91-1 59101-30-3 68459-80-3 75951-38-1 75951-39-2 75980-64-2

RL: CAT (Catalyst use); USES (Uses)

(catalysts, storage-stable halogenated polyols containing, for polyurethane foam manufacture)

T 76199-08-1P

RL: PEP (Physical, engineering or chemical process); PREP (Preparation); PROC (Process)

(cellular, manufacture of, chlorinated polyether polyols for, storage-stable acid-blocked amine catalysts for)

- L6 ANSWER 5 OF 6 CAPLUS COPYRIGHT 2009 ACS on STN
- AN 1979:138618 CAPLUS
- DN 90:138618
- OREF 90:22001a,22004a
- ED Entered STN: 12 May 1984
- TI Catalytically stable polyol mixture for manufacturing polyurethane foams
- IN Fuzesi, Stephen PA Olin Corp., USA
- PA Olin Corp., USA SO Ger. Offen., 23 pp.
- CODEN: GWXXBX
- DT Patent
- LA German
- IC C08G018-32
- CC 36-6 (Plastics Manufacture and Processing)

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PI	DE 2822819		A1	19781207	DE 1978-2		19780524
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	BR 7803348		A	19790116	BR 1978-3	348	19780526
	JP 53149299		A	19781226	JP 1978-6	4854	19780530
	JP 61041928		В	19860918			
	FR 2393024		A1	19781229	FR 1978-1	6143	19780530
	FR 2393024		B1	19820625			
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C08G0018-50 [I,A]; C08G0065-00 [I,C*]; C08G0065-26

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                        [ICS,C*]
                 IPCR
                        C08G0018-00 [I,A]; C08G0018-00 [I,C*]; C08G0018-18
                        [I,A]; C08G0018-30 [I,A]; C08G0018-32 [I,A];
                        C08G0018-50 [I,A]; C08G0065-00 [I,C*]; C08G0065-26
                        [I, A]
                 ECLA
                        C08G018/18R; C08G018/50C3; C08G065/26C1
 JP 53149299
                 IPCI
                        C08G0018-14 [ICM]; C08G0018-18 [ICA]; C08G0018-00
                        [ICA,C*]
                 TPCR
                        C08G0018-00 [I,A]; C08G0018-00 [I,C*]; C08G0018-18
                        [I,A]; C08G0018-30 [I,A]; C08G0018-32 [I,A];
                        C08G0018-50 [I,A]; C08G0065-00 [I,C*]; C08G0065-26
                        [I, A]
FR 2393024
                 IPCI
                        C08L0071-00 [ICM]; C08G0018-14 [ICS]; C08K0005-17
                        [ICS]; C08K0005-00 [ICS,C*]
                 IPCR
                        C08G0018-00 [I,A]; C08G0018-00 [I,C*]; C08G0018-18
                        [I,A]; C08G0018-30 [I,A]; C08G0018-32 [I,A];
                        C08G0018-50 | I.Al; C08G0065-00 | I.C*|; C08G0065-26
                        [I.A]
AB
    Catalytically stable polyol mixts. for the preparation of polyurethane foams
     comprised a halogenated polyol with an acid-blocked amine as catalyst.
     Thus, a resin [69620-14-0] foam prepared by mixing a halogenated polyol
     (prepared by condensation of 4,4,4-trichloro-1,2-epoxybutane with an
     equimol. mixture of ethylene glycol and α-D-glucose monohydrate) 100,
     an addnl. polyol (caprolactone-glycerin copolymer) 20, a wetting agent 2,
     trimethylbutanediamine monoformate [69418-55-9] catalyst 5, blowing agent
     36, and PAPI 117.5 parts had cream formation time 14 s, gel formation time
     72 s, time to freedom from tackiness 105 s, and foam formation time 130 s.
ST
     amine catalyst polyurethane foam
ΙT
     Polymerization catalysts
        (acid-blocked amines, for polyurethane foams)
     Urethane polymers, preparation
     RL: PREP (Preparation)
        (manufacture of cellular, acid-blocked amines as catalysts for)
                 68459-80-3 69418-55-9
                                           69418-56-0
     RL: CAT (Catalyst use); USES (Uses)
        (catalysts, for polyurethane foam manufacture)
IT
     69620-14-0P
     RL: PREP (Preparation)
        (manufacture of cellular, catalysts for)
    ANSWER 6 OF 6 CAPLUS COPYRIGHT 2009 ACS on STN
L6
    1976:464918 CAPLUS
AN
DN
     85:64918
OREF 85:10443a,10446a
ED
    Entered STN: 12 May 1984
ΤI
    Epoxy group-containing, quaternary ammonium salt-containing resins
TN
    Bosso, Joseph F.; Wismer, Marco
PA
    PPG Industries, Inc., USA
    U. S. Publ. Pat. Appl. B, 12 pp.
    CODEN: USXXDP
    Patent
LA.
    English
TC
    CORG
INCL 260029200EP
```

42-7 (Coatings, Inks, and Related Products)

FAN.CNT 12 PATENT NO.		KIND	DATE		PLICATION NO.	DATE
PI US 455686		15	19760302		1974-455686	19740328
US 4001156 FR 2051662 US 4001101		A A5 A	19770104 19710409 19770104	US	1970-25584 1971-167470	19700709 19710729
FR 2118887 FR 2118887		A6 A2	19720804 19720804		1971-29442	19710811
DE 2142449 DE 2142449		A C2	19720629 19820519	DE	1971-2142449	19710825
AT 321430 US 3839252 US 4191674 PRAI US 1968-77 US 1969-84 US 1970-56 US 1970-10 US 1970-10 US 1971-12 US 1971-15 US 1971-16 US 1971-17 US 1971-17 US 1971-17 US 1971-17	0847 0848 730 0825 0834 9267 8063 7470 7697	B A A3 A2 A2 A2 A2 A2 A2 A2 A2 A2 A2	19750325 19741001 19800304 19681031 19690710 19700720 19701222 19701222 19710329 19710629 19710729 19720803 19710729	US	1971–10973 1972–277007 1977–844944	19711221 19720801 19771025
US 1975-59 CLASS	9260	A2	19750725			
PATENT NO.					CATION CODES	
US 455686	IC INCL IPCI IPCR	C08G005 [I,A]; C08G005	51-24 [ICM] 59-00 [I,C*] C08G0059-52	[I,	8G0059-40 [I,A]; A]; C08G0059-58 D0005-44 [I,C*];	I,A];
	NCL	523/421	1.000; 523/4	14.0	00; 024/704.100; 00; 523/416.000; 00; 528/121.000;	523/417.000;
	ECLA	C08G059		059/	50; C08G059/52; C	
FR 2051662	IPCI	C23B001		C08	G0033-00 [ICS]; 0	08G0030-00
	IPCR	C08G005	59-00 [I,C*] C08G0059-52	; C0	8G0059-00 [I,A]; A]; C08G0059-64 9D0005-44 [I,A]	
US 4001101	IPCI IPCR	C25D003 C08G005 [I,A];	13-06 [ICM]; 59-00 [I,C*] C08G0059-52	C25 ; C0	D0013-04 [ICM,C*] 8G0059-40 [I,A]; A]; C08G0059-58 D0005-44 [I,C*];	C08G0059-50 [I,A];
	NCL ECLA	204/502 C08G059	2.000; 523/4 9/40B5; C08G 9/64; C09D00	059/	50; C08G059/52; C	08G059/58;
FR 2118887	IPCR	C08G005	59-00 [I,C*] C08G0059-58	; C0	D4K 8G0059-40 [I,A]; A]; C09D0005-44	
DE 2142449	ECLA IPCI IPCR	C08G005 C08G005 C08G005 [I,A];	59-14 [ICM]; 59-00 [I,C*]	C08	50; C08G059/58; C G0059-00 [ICM,C*] 8G0059-40 [I,A]; A]; C09D0005-44	C08G0059-50

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ECLA
                       C08G059/40B5; C08G059/50; C08G059/58; C09D005/44D4B
 AT 321430
                 TPCT
                       C23B0013-00 [ICM]
                 IPCR
                       C25D0013-04 [I,C*]; C25D0013-06 [I,A]
IIS 3839252
                 IPCI
                       C08B0013-00 [ICM]; C08G0030-16 [ICS]; C08G0051-24 [ICS]
                 IPCR
                       C09D0005-44 [I,C*]; C09D0005-44 [I,A]
                 NCL
                        523/414.000; 204/501.000; 523/402.000; 523/417.000;
                        523/420.000; 523/421.000; 523/426.000; 528/219.000
                 ECLA
                       C09D005/44D4B
                       C25D0013-06 [ICM]; C25D0013-04 [ICM,C*]
US 4191674
                 IPCI
                 IPCR
                       C09D0005-44 [I,C*]; C09D0005-44 [I,A]
                 NCL
                       525/327.300; 523/414.000; 524/901.000; 525/379.000;
                       525/531.000: 528/112.000
                 ECLA
                       C09D005/44K
AB
    The title resins, useful as water-dispersible electrophoretic coatings,
     are prepared by reaction of polyepoxides with 1-50 phr amine salt at
     70-100° in the presence of 1.75-20% H2O and adding B(OH)3
     [11113-50-1] or a hydrolyzable derivative Thus, heating 1770 parts Epon 829
     (epoxy resin) [37325-21-6] and 302 parts bisphenol A 45 min at
     180-5° gives a resin with epoxy equivalent 330-50. Heating this resin
     500, 75% 2-(dimethylamino)ethanol lactate (salt) 105, and H20 24.3 parts
     62 min at 92-102° gives a resin, epoxy equivalent 1050, OH number 338,
     quaternary ammonium lactate content 0.666 meguiv./q solids, Gardner-Holdt
     viscosity of 50% EtOCH2CH2OH solution H-I. Diluting 100 parts resin with H2O
t o
     10% solids, adding 100 parts 4.5% aqueous B(OH)3, coating on Al panels for 30
     sec at 150 V and 77°F, and baking 30 min at 350°F gives a
     hard, glossy, Me2CO-resistant film. In the absence of B(OH)3, the film is
     soft.
ST
     epoxy resin coating electrophoretic; dimethylaminoethanol lactate epoxy
     coating; boric acid epoxy coating
     Quaternary ammonium compounds, uses and miscellaneous
     RL: USES (Uses)
        (epoxy resin coatings containing, electrophoretic)
     Coating materials
        (epoxy resin-alkanolamine salt reaction products, electrophoretic,
        containing boric acid)
     Formic acid, compound with 2-(dimethylamino)ethanol (1:1), reaction products
        with epoxy resins
     Oxirane, (chloromethyl)-, polymer with
        4,4'-(1-methylethylidene)bis[phenol], reaction products with
        (dimethylamino)ethanol salts
     Phenol, 4,4'-(1-methylethylidene)bis-, polymer with (chloromethyl)oxirane,
       reaction products with (dimethylamino)ethanol salts
     Propanoic acid, 2-hydroxy-, compound with 2-(dimethylamino)ethanol (1:1),
        reaction products with epoxy resins
     RL: TEM (Technical or engineered material use); USES (Uses)
        (coatings, electrophoretic, containing boric acid derivs.)
     56669-87-5D, Ethanol, 2-(dimethylamino)-, 2-hydroxypropanoate (salt),
     reaction products with epoxy resins 59101-30-3D, Ethanol,
     2-(dimethylamino)-, formate (salt), reaction products with epoxy resins
     RL: TEM (Technical or engineered material use); USES (Uses)
        (coatings, electrophoretic, containing boric acid derivs.)
     10043-35-3 36711-54-3
     RL: USES (Uses)
        (epoxy resin electrophoretic coatings containing)
=> s (dimethylaminoethanol or dimethylamino ethanol) and (formic or formate)
          2798 DIMETHYLAMINOETHANOL
         77799 DIMETHYLAMINO
```

324073 ETHANOL

1061 DIMETHYLAMINO ETHANOL

```
(DIMETHYLAMINO(W)ETHANOL)
         57184 FORMIC
         45920 FORMATE
            56 (DIMETHYLAMINOETHANOL OR DIMETHYLAMINO ETHANOL) AND (FORMIC OR
               FORMATE)
=> s ionic and 17
        304581 IONIC
L8
             0 IONIC AND L7
=> d his
     (FILE 'HOME' ENTERED AT 12:57:44 ON 19 MAR 2009)
     FILE 'REGISTRY' ENTERED AT 12:58:22 ON 19 MAR 2009
                E N, N-DIMETHYLETHANOLAMMONIUM FORMATE/CN
                E E2
              1 S E3
L1
     FILE 'CAPLUS' ENTERED AT 13:01:52 ON 19 MAR 2009
              1 S US20070185330/PN
L2
1.3
              2 S DIMETHYLETHANOLAMMONIUM AND FORMATE
     FILE 'CAPLUS' ENTERED AT 13:15:01 ON 19 MAR 2009
     FILE 'REGISTRY' ENTERED AT 13:15:11 ON 19 MAR 2009
T. 4
              2 S 59101-30-3/RN OR 53518-18-6/RN
     FILE 'CAPLUS' ENTERED AT 13:16:40 ON 19 MAR 2009
                S 59101-30-3/REG#
    FILE 'REGISTRY' ENTERED AT 13:18:46 ON 19 MAR 2009
1.5
              1 S 59101-30-3/RN
    FILE 'CAPLUS' ENTERED AT 13:18:47 ON 19 MAR 2009
L6
             6 S L5
L7
             56 S (DIMETHYLAMINOETHANOL OR DIMETHYLAMINO ETHANOL) AND (FORMIC O
L8
              0 S IONIC AND L7
=> s 17 not 16
           55 L7 NOT L6
1.9
=> d 1-55 all
1.9
    ANSWER 1 OF 55 CAPLUS COPYRIGHT 2009 ACS on STN
AN
    2009:140081 CAPLUS
DN
    150:214372
    Entered STN: 05 Feb 2009
ED
     Preparation of 2-aminobenzothiazole derivatives as phosphoinositide
ΤI
     3-kinase (PI3 kinase) modulators
     Booker, Shon; D'Angelo, Noel; D'Amico, Derin C.; Kim, Tae-Seong; Liu,
     Longbin; Meagher, Kristin; Norman, Mark H.; Panter, Kathleen; Schenkel,
     Laurie B.; Smith, Adrian L.; Tamavo, Nuria A.; Whittington, Douglas A.;
    Xi, Ning; Yang, Kevin
PΑ
    Amgen Inc., USA
SO
    PCT Int. Appl., 279pp.
    CODEN: PIXXD2
    Patent
```

28-7 (Heterocyclic Compounds (More Than One Hetero Atom))

LA.

FAN.CNT 1

English

Section cross-reference(s): 1

									APPLICATION NO.									
ΡI	WO							20090205								200808		301
		W:				AM,												
			CA,	CH,	CN,	CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DO,	DZ,	EC,	EE,	EG,	ES,
			FΙ,	GB,	GD,	GE,	GH,	GM,	GT,	HN,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	KE,
						KP,												
						MN,												
						RS,											SY,	TJ,
						TT,												
		RW:				CH,												
						LT,												
						CF,												
						GM,						SD,	SL,	SZ,	TZ,	UG,	ZM,	ZW,
						KG,												
		2009									US 2	008-	2214	16		2	0080	301
		2007	-963	263P		P		2007	0802									
CLAS		NO.		OT 3	00	D3 mE1	.m. =		v 01		DTO3	m T ON	con					
		NO.		CLA		PAIE	AT E	AMIL	Y CL.	4551	FICA	TION	COD	<u></u>				
WO	2009	90178	22	IPC	I	C07D	0277	-82	[I,A]; C	07D0	277-] 00	I,C*]; C	07D0	413-) 4
						[I,A]; C07D0413-00 [I,C*]; C07D0417-04 [I,A];												
						C07D	0417	-14	[I,A]; C	07D0	417-] 00	I,C*]; C	07D0	513-) 4
								07D0										
						A61K	0031	-424	[I,	A];	A61K	0031	-428	[I,	A]; ;	A61K	0031	-429
						[I,A]												
US	2009	90054	405	IPC:		A61K)
						[I,A]												
						C07D												
								61KO								5 [I	,C*]	;
						A61K												
				NCL		514/2												
						540/	597.	000;	514	/256	.000	; 51	4/23	5.80	0; 5	14/2	55.0	50
GI																		

AB The title compds. [I, Al, A2, A3, A4 = (un)substituted CH or N, provided that no more than two of A1, A2, A3 and A4 is N; X = O or S; R1 = H, C1-6 alkyl, C2-6 alkenyl, C2-6 alkynyl, or C3-6 cycloalkyl, R2 = C1-6 each optionally substituted alkyl-R7a, C2-6 alkynyl-R7a, C2-6 alkynyl-R7a, or C3-6 cycloalkyl-R7a, C(O)R7a, C(O)NHR7a, CO2R7a, S(O)2R7a or a partially or fully saturated or fully unsatd. 5- or 6-membered monocyclic ring formed of carbon atoms and including 1-3 heteroatoms selected from N, O and S; R7a = H, each optionally substituted C1-8 alkyl, C2-8 alkenyl, C2-8 alkynyl, C3-6 cycloalkyl, or C4-8 cycloalkenyl, NRBR9, NRSP9, ORS, SRB, ORS, SR9, C(O)RB, OC(O)R9, COOR9, C(O)R9, C(O)NRBR9, NRSC(O)R9, C(O)NRSP9, NRSC(O)R9, S(O)2RB, S(O)2R9, S(O)2RB, S(O)2R9, S(O)2RB, OC(O)R9, S(O)2RB, OC(O)R9, R8 a partially or fully saturated or unsatd. 3-8 membered monocyclic or 6-12 membered bicyclic ring system, said ring system formed of carbon atoms optionally including 1-3 heteroatoms if

```
monocyclic or 1-6 heteroatoms if bicyclic, said heteroatoms selected from
O, N, or S, if bicyclic, said heteroatoms selected from O, N, or S, etc.]
or pharmaceutically acceptable salts thereof were prepared. The present
invention comprises a new class of compds. capable of modulating the
activity of PI3 kinase and, accordingly, useful for treatment of PI3
kinase-mediated diseases, including melanomas, leukemias, glioblastomas,
carcinomas and other cancer-related conditions. Thus, 0.0683 q
N-[6-[6-chloro-5-[(2-methoxyethoxy)methoxy]pyridin-3-yl]-1,3-benzothiazol-
2-vllacetamide was treated with 5 mL TFE (2,2,2-trifluoroethanol)(sic) and
2.0 M HCl (0.251 mL) at reflux in a 120° oil bath for 45 min. The
reaction mixture was cooled, evaporated in vacuo, suspended in ethanol, heated
with a 120° oil bath, cooled, evaporated, dissolved in dry pyridine,
stirred with 5 A activated mol. sieves for 1 h, filtered, treated with
Ac20, and heated using a 70° coil bath for 5 h to give
5-(2-acetamido-1,3-benzothiazo1-6-y1)-2-chloropyridin-3-y1 acetate (II)
(0.0314 g, 51.8% yield). II showed IC50 of 0.0020, 0.0122, and 0.0017
μg/mL against PI3α, PI3β, and HCT 116 human colon carcinoma
cell line, resp.
PI3 kinase modulator; aminobenzothiazole prepn phosphoinositide 3 kinase
modulator
Neuroglia, neoplasm
   (glioblastoma; preparation of 2-aminobenzothiazole derivs. as PI3 kinase
Human
Leukemia
   (preparation of 2-aminobenzothiazole derivs. as PI3 kinase modulators)
Antitumor agents
Carcinoma
Melanoma
Neoplasm
   (preparation of 2-aminobenzothiazole derivs. as PI3 kinase modulators for
   treatment of PI3 kinase mediated diseases including melanomas,
   carcinomas, and other cancer-related conditions)
1112980-55-8P, N-[6-[6-Chloro-5-[(1-methylethyl)amino]-3-pyridinyl]-1,3-
benzothiazol-2-vllacetamide
                             1112980-65-0P,
N-[6-(5-Amino-6-methyl-3-pyridinyl)-1,3-benzothiazol-2-yl]acetamide
1112980-79-6P, N-[5-(3-Aminophenyl)-[1,3]thiazolo[5,4-b]pyridin-2-
yl]acetamide 1112982-49-6P, 5-(1,3-Benzothiazol-6-yl)-2-chloro-3-
            1112982-50-9P, 5-(1,3-Benzothiazol-6-yl)-2-chloropyridin-3-yl
pyridinol
acetate
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic
preparation); THU (Therapeutic use); BIOL (Biological study); PREP
(Preparation); RACT (Reactant or reagent); USES (Uses)
   (intermediate; preparation of 2-aminobenzothiazole derivs. as PI3 kinase
   modulators)
433-14-7P, 4-Fluoro-N-methylbenzenesulfonamide
                                                1216-97-3P,
N-(5-Bromopyridin-3-v1)-4-methylbenzenesulfonamide
                                                    2922-45-4P,
                       7010-86-8P, 4-Methoxy-N-methylbenzenesulfonamide
3-Pvridinesulfonamide
15864-32-1P 16628-26-5P, N-(6-Bromo-1,3-benzothiazol-2-v1)acetamide
20358-05-8P, 7-Bromobenzo[d]thiazol-2-amine
                                            23451-95-8P.
2-Amino-5-bromobenzenethiol
                             35088-84-7P,
N-Ethyl-4-methoxybenzenesulfonamide
                                     53218-26-1P, 6-Bromobenzo[d]thiazole
70232-59-6P, 5-Bromo-N-methyl-3-nitropyridin-2-amine
                                                      75104-92-6P,
6-Bromo-N-methylbenzo[d]thiazol-2-amine 89415-54-3P.
5-Bromo-N-methylpyridine-2,3-diamine 173020-15-0P,
N-Methyl-3-methylbenzenesulfonamide 179626-68-7P,
2-(tert-Butoxycarbonylamino)-4-benzothiazole-6-carbohydrazide
188057-49-0P
              214911-10-1P, 6-Fluoro-2-iodopyridin-3-o1 476280-90-7P,
N-(6-Bromo-1,3-benzothiazo1-2-y1)cyclohexanecarboxamide 851169-58-9P,
2-Fluoro-N-methylbenzenesulfonamide
                                    873383-06-3P,
5-Bromo-N-methylpyridin-3-amine 885069-14-7P,
```

N-[6-(4,4,5,5-Tetramethyl-1,3,2-dioxaborolan-2-yl)-1,3-benzothiazol-2-

ST

```
yl]acetamide
              911434-04-3P, Diethyl
2-(5-bromo-3-nitropyridin-2-v1)malonate
                                        911434-05-4P.
5-Bromo-2-methyl-3-nitropyridine 914358-73-9P,
5-Bromo-2-methylpyridin-3-amine 947248-67-1P,
N-(6-Bromo-4-fluoro-1.3-benzothiazo1-2-v1)acetamide 1002309-47-8P.
6-(4,4,5,5-Tetramethyl-1,3,2-dioxaborolan-2-yl)-1,3-benzothiazole
1112982-56-5P, 2-Chloro-6-(2-fluorophenylthio)pyridine
                                                       1112982-57-6P.
2-Chloro-6-(2-fluorophenylsulfonyl)pyridine
                                             1112982-59-8P,
2-Chloro-6-(4-fluorophenvlsulfonvl)pyridine
                                             1112982-61-2P,
2-Chloro-6-(4-methoxyphenylthio)pyridine 1112982-62-3P.
2-Chloro-6-(4-methoxyphenylsulfonyl)pyridine 1112982-63-4P,
N-(6-Chloropyridin-2-y1)benzenesulfonamide
                                           1112982-65-6P.
N-[6-(6-Aminopyridin-2-yl)-1,3-benzothiazol-2-yl]acetamide
1112982-66-7P, N-(6-Chloropyridin-2-yl)-N-methyl-4-
methylbenzenesulfonamide 1112982-68-9P,
N-(7-Bromo-1,3-benzothiazol-2-vl)acetamide
                                            1112982-69-0P.
4-Bromo-2-(4-fluorophenylthio)thiazole 1112982-70-3P,
4-Bromo-2-(4-fluorophenylsulfonyl)thiazole 1112982-71-4P,
N-Acetyl-N'-(4-bromo-2,6-difluorophenyl)thiourea 1112982-72-5P,
N-[4-Fluoro-6-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-1,3-
benzothiazol-2-vllacetamide 1112982-73-6P,
5-Bromo-2-chloro-N-isopropylpyridin-3-amine
                                             1112982-74-7P,
5-Bromo-N'-isopropyl-N-methylpyridine-2,3-diamine 1112982-75-8P.
6-Bromo-2, 2, 3-trimethyl-2, 3-dihydro-1H-imidazo[4, 5-b]pyridine
1112982-76-9P, N-(5-Bromothiazolo[5,4-b]pvridin-2-vl)acetamide
1112982-77-0P, N-(5-Bromo-2-chloropyridin-3-yl)-4-(2-hydroxypropan-2-
vl)benzenesulfonamide 1112982-79-2P,
3-[N,N-Bis(4-fluorophenylsulfonyl)amino]-5-bromo-2-chloropyridine
1112982-80-5P, N-[6-[6-Chloro-5-[N,N-bis[(4-fluorophenyl)sulfonyl]amino]-3-
pyridinyl]-1,3-benzothiazol-2-yl]acetamide
                                           1112982-81-6P.
N-(5-Bromo-2-chloropyridin-3-yl)-4-methoxybenzenesulfonamide
1112982-82-7P, N-(5-Bromo-2-chloropyridin-3-yl)-N-(4-
methoxyphenylsulfonyl)-4-methoxybenzenesulfonamide
                                                   1112982-83-8P,
Pentafluorophenyl 2-(tert-butoxycarbonyl)-1,3-benzothiazole-6-carboxylate
               1112982-86-1P
1112982-85-0P
                               1112982-87-2P,
N-(5-Bromo-2-chloropyridin-3-yl)cyclohexanesulfonamide
                                                       1112982-88-3P.
N-[6-(5-Amino-6-chloropyridin-3-y1)-1,3-benzothiazo1-2-y1]acetamide
1112982-89-4P, N-[6-(2-Chloropyridin-4-yl)-1,3-benzothiazol-2-yl]acetamide
1112982-90-7P, N-(5-Bromopyridin-3-yl)-N-methyl-4-
(trifluoromethyl)benzenesulfonamide 1112982-91-8P,
N-(6-Chloropyridin-2-vl)-N-methyl-3-methylbenzenesulfonamide
1112982-92-9P, N-(5-Bromopyridin-3-vl)-4-fluorobenzenesulfonamide
1112982-94-1P, 1-[2-[(5-Bromopyridin-3-yl)oxy]ethyl]pyrrolidin-2-one
1112983-05-7P, 5-Bromo-2-iodo-3-[(2-methoxyethoxy)methoxy]pyridine
1112983-06-8P, 5-Bromo-2-chloro-3-[(2-methoxyethoxy)methoxy]pyridine
1112983-08-0P, 2-[(5-Bromo-2-chloropyridin-3-yl)oxy]propanenitrile
1112983-11-5P, 2-[(5-Bromopyridin-3-v1)oxylacetonitrile
                                                        1112983-13-7P.
2-[(5-Bromo-2-chloropyridin-3-yl)oxy]acetonitrile
                                                  1112983-14-8P.
2-[(5-Bromopyridin-3-yl)oxy]ethanamine hydrochloride 1112983-17-1P,
                                        1112983-18-2P,
2-[(5-Bromopyridin-3-yl)oxy]ethanamine
N-[2-[(5-Bromopyridin-3-yl)oxy]ethyl]-2-methoxyacetamide
                                                          1112983-19-3P,
1-[[(5-Bromopyridin-3-v1)oxy]methyl]cyclopropanamine 1112983-20-6P,
(R)-5-[[(5-Bromopyridin-3-v1)oxy]methyl]pyrrolidin-2-one
                                                          1112983-21-7P,
6-[6-(3-Azabicyclo[3.2.2]nonan-3-yl)pyrazin-2-yl]benzo[d]thiazol-2-amine
1112983-22-8P, N-[6-(4,4,5,5-Tetramethyl-1,3,2-dioxaborolan-2-yl)-1,3-
benzothiazo1-2-y1]cyclohexanecarboxamide 1112983-23-9P,
N-[2-Chloro-5-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)pyridin-3-yl]-4-
methoxybenzenesulfonamide
                          1112983-24-0P,
6-Bromo-N-isopropylbenzo[d]thiazo1-2-amine
                                           1112983-25-1P,
6-Bromo-N-(cyclohexylmethyl)-1,3-benzothiazol-2-amine 1112983-26-2P,
N-(5-Bromo-2-chloropyridin-3-y1)-3-(difluoromethoxy)benzenesulfonamide
1112983-27-3P, N-[2-Chloro-5-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-
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N-(5-Bromo-2-chloropyridin-3-y1)piperidine-1-sulfonamide 1112983-29-5P,
N-Methyl-6-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-1,3-benzothiazol-
         1112983-31-9P, N-[2-Chloro-5-(4,4,5,5-tetramethyl-1,3,2-
dioxaborolan-2-vl)pvridin-3-vl1-4-fluorobenzenesulfonamide
1112983-33-1P, 6-[6-Chloro-5-[(2-methoxyethoxy)methoxy]pyridin-3-y1]-1,3-
benzothiazole 1112983-34-2P, 6-Fluoro-2-iodo-3-[(2-
methoxyethoxy)methoxy|pyridine 1112983-35-3P,
6-Fluoro-3-I(2-methoxyethoxy)methoxyl-2-(trifluoromethyl)pyridine
1112983-36-4P, 6-Fluoro-4-iodo-3-1(2-methoxyethoxy)methoxyl-2-
(trifluoromethyl)pyridine 1112983-37-5P.
2-Fluoro-3-iodo-5-[(2-methoxyethoxy)methoxy]-6-(trifluoromethyl)pyridine
1112983-39-7P, 2-Fluoro-3, 4-diiodo-5-[(2-methoxyethoxy)methoxy]-6-
(trifluoromethyl)pyridine 1112983-40-0P,
6-[2-Fluoro-5-[(2-methoxyethoxy)methoxy]-6-(trifluoromethyl)pyridin-3-yl]-
2-methylbenzo[d]thiazole 1113041-99-8P 1113042-01-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
   (intermediate; preparation of 2-aminobenzothiazole derivs. as PI3 kinase
   modulators)
1112983-41-1P
               1112983-42-2P
                               1112983-43-3P
                                               1112983-44-4P
1112983-45-5P
               1112983-46-6P
                               1112983-48-8P
                                               1112983-49-9P
1112983-50-2P
               1112983-51-3P
                               1112983-52-4P
                                               1112983-53-5P
1112983-54-6P
               1112983-55-7P
                               1112983-56-8P
                                               1112983-57-9P
1112983-58-0P
               1112983-59-1P
                               1112983-61-5P
                                               1112983-62-6P
1112983-63-7P
               1112983-64-8P
                               1112983-65-9P
                                               1112983-66-0P
1112983-67-1P
               1112983-68-2P
                               1112983-69-3P
                                               1112983-70-6P
1112983-71-7P
               1112983-72-8P
                               1112983-73-9P
                                               1112983-75-1P
1112983-76-2P
               1112983-77-3P
                               1112983-78-4P
                                               1112983-79-5P
1112983-80-8P
               1112983-81-9P
                               1112983-83-1P
                                               1112983-84-2P
1112983-85-3P
               1112983-86-4P
                               1112983-87-5P
                                               1112983-89-7P
                               1112983-92-2P
1112983-90-0P
               1112983-91-1P
                                               1112983-93-3P
1112983-94-4P
               1112983-96-6P
                               1112983-97-7P
                                               1112983-98-8P
1112983-99-9P 1112984-00-5P
                               1112984-01-6P
                                               1112984-02-7P
1112984-03-8P 1112984-04-9P
                               1112984-05-0P
                                               1112984-08-3P
1112984-09-4P 1112984-10-7P
                              1112984-11-8P 1112984-12-9P
1112984-13-0P 1112984-14-1P
                              1112984-15-2P 1112984-16-3P
1112984-18-5P 1112984-19-6P
                              1112984-20-9P
                                              1112984-21-0P
1112984-22-1P 1112984-23-2P 1112984-24-3P
                                               1112984-25-4P
1112984-26-5P 1112984-27-6P 1112984-28-7P
                                               1112984-29-8P
                                               1112984-33-4P
1112984-30-1P 1112984-31-2P 1112984-32-3P
1112984-34-5P 1112984-35-6P 1112984-36-7P
RL: PAC (Pharmacological activity); PRPH (Prophetic); SPN (Synthetic
preparation); THU (Therapeutic use); BIOL (Biological study); PREP
(Preparation); USES (Uses)
   (preparation of 2-aminobenzothiazole derivs. as PI3 kinase modulators)
1112980-92-3P, N-[5-(2-Amino-1,3-benzothiazol-6-v1)-1,3,4-oxadiazol-2-v1]-
4-fluorobenzenesulfonamide
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic
preparation); THU (Therapeutic use); BIOL (Biological study); PREP
(Preparation); RACT (Reactant or reagent); USES (Uses)
   (preparation of 2-aminobenzothiazole derivs. as PI3 kinase modulators)
1112979-13-1P, N-[6-[2-[3-(3-Pyridinyl)propoxy]-4-pyrimidinyl]-1,3-
benzothiazol-2-vllacetamide 1112979-14-2P.
N-[6-[2-[(3-Pyridinyl)methoxy]-4-pyrimidinyl]-1,3-benzothiazol-2-
vllacetamide
              1112979-16-4P, N-[6-[2-[(Benzyl)oxy]-4-pyrimidinyl]-1,3-
benzothiazol-2-yl]acetamide 1112979-17-5P,
N-[6-[2-(3-Phenylpropoxy)-4-pyrimidinyl]-1,3-benzothiazol-2-yl]acetamide
1112979-18-6P, N-[6-[2-(3-Methoxypropoxy)-4-pyrimidiny1]-1,3-benzothiazol-
                1112979-19-7P, N-[6-[2-(1-Methylethoxy)-4-pyrimidinyl]-
2-vllacetamide
1,3-benzothiazo1-2-y1]acetamide 1112979-20-0P,
N-[6-[2-(2-Phenylethoxy)-4-pyrimidiny1]-1,3-benzothiazol-2-y1]acetamide
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ΤТ

ΙT

yl)pyridin-3-yl]-3-(difluoromethoxy)benzenesulfonamide 1112983-28-4P,

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1112979-21-1P, N-[6-[2-(3-Dimethylaminopropoxy)-4-pyrimidinyl]-1,3-
benzothiazo1-2-v1|acetamide 1112979-22-2P,
N-[6-[2-(2-Dimethylaminoethoxy)-4-pyrimidinyl]-1,3-benzothiazol-2-
             1112979-23-3P, N-[6-[2-(3-Morpholinopropoxy)-4-pyrimidinyl]-
vllacetamide
1.3-benzothiazol-2-vllacetamide 1112979-24-4P.
N-[6-[2-(2-Morpholinoethoxy)-4-pyrimidiny1]-1,3-benzothiazol-2-
             1112979-25-5P, N-[6-[2-[(3-Fluorobenzyl)oxy]-4-pyrimidinyl]-
vllacetamide
1,3-benzothiazol-2-yl]acetamide 1112979-26-6P,
N-[6-(2-Benzvl-4-pyrimidinvl)-1,3-benzothiazol-2-vl]acetamide
1112979-27-7P, N-[6-[2-(3-Phenylpropyl)-4-pyrimidinyl]-1,3-benzothiazol-2-
yl]acetamide 1112979-28-8P, N-[6-[2-(2-Phenylethyl)-4-pyrimidinyl]-1,3-
benzothiazol-2-vllacetamide 1112979-29-9P.
N-[6-[2-[(4-Methoxyphenyl)sulfanyl]-4-pyrimidinyl]-1,3-benzothiazol-2-
v1]acetamide 1112979-30-2P, N-[6-[2-[(4-Pyridiny1)methoxy]-4-
pyrimidinyl]-1,3-benzothiazol-2-yl]acetamide 1112979-31-3P,
N-[6-[2-[2-(3-Pyridinyl)ethoxy]-4-pyrimidinyl]-1,3-benzothiazol-2-
yl]acetamide 1112979-32-4P, N-[6-[2-(Benzylsulfanyl)-4-pyrimidinyl]-1,3-
benzothiazol-2-yl]acetamide
                            1112979-34-6P,
N-[6-[2-[3-(1H-1,2,3-Triazol-1-yl)propoxy]-4-pyrimidinyl]-1,3-benzothiazol-
2-yl]acetamide 1112979-35-7P, N-[6-[2-(Phenylsulfanyl)-4-pyrimidinyl]-
1,3-benzothiazo1-2-y1]acetamide 1112979-36-8P,
N-[6-[2-[(6-Ouinolinv1)methoxy]-4-pyrimidinv1]-1,3-benzothiazol-2-
vllacetamide
             1112979-37-9P, N-[6-[2-[(2-Fluorophenvl)sulfanvl]-4-
pyrimidinyl]-1,3-benzothiazol-2-yl]acetamide
                                             1112979-38-0P.
N-[6-[2-[(1H-Indol-5-yl)methoxy]-4-pyrimidinyl]-1,3-benzothiazol-2-
             1112979-41-5P, N-[6-[2-[(1-Methyl-4-piperidinyl)methoxy]-4-
vllacetamide
pyrimidinyl]-1,3-benzothiazol-2-vl]acetamide
                                             1112979-43-7P,
N-[6-[2-[(4-Fluorophenv1)sulfanv1]-4-pvrimidinv1]-1,3-benzothiazol-2-
vllacetamide
             1112979-45-9P, N-[6-[2-[(4-Methoxy-2-methylphenyl)sulfanyl]-
4-pyrimidinyl]-1,3-benzothiazol-2-yl]acetamide 1112979-47-1P,
N-[6-[2-[(2-Methoxyphenyl)sulfanyl]-4-pyrimidinyl]-1,3-benzothiazol-2-
              1112979-48-2P, N-[4-[[4-[2-(Acetylamino)-1,3-benzothiazol-6-
yl]acetamide
v1]-2-pyrimidinyl]sulfanyl]phenyl]acetamide
                                            1112979-49-3P,
N-[6-[2-[(2-tert-Butylphenyl)sulfanyl]-4-pyrimidinyl]-1,3-benzothiazol-2-
yl]acetamide 1112979-51-7P, N-[6-[2-[(1-Methyl-4-piperidinyl)oxy]-4-
pyrimidinyl]-1,3-benzothiazol-2-yl]acetamide
                                             1112979-52-8P.
N-[6-[2-[3-(2-0xo-1,3-oxazolidin-3-y1)propoxy]-4-pyrimidinyl]-1,3-
benzothiazol-2-yl]acetamide
                            1112979-53-9P,
N-[6-(2-Phenoxy-4-pyrimidinyl)-1,3-benzothiazol-2-yl]acetamide
1112979-54-0P, N-[6-[2-[(2-Methylphenyl)sulfanyl]-4-pyrimidinyl]-1,3-
benzothiazol-2-vllacetamide
                             1112979-55-1P,
N-[6-[2-[(3-Methylphenyl)sulfanyl]-4-pyrimidinyl]-1,3-benzothiazol-2-
yl]acetamide
             1112979-56-2P, N-[6-[2-[(4-Methylphenyl)sulfanyl]-4-
pyrimidinyl]-1,3-benzothiazol-2-yl]acetamide
                                             1112979-57-3P,
N-[6-[2-[(2-Methylbenzyl)sulfanyl]-4-pyrimidinyl]-1,3-benzothiazol-2-
vl]acetamide
              1112979-58-4P, N-[6-[2-[(4-Methoxybenzyl)oxy]-4-
pyrimidinyl]-1,3-benzothiazol-2-vl]acetamide
                                             1112979-59-5P,
N-[6-[2-[(4-Fluorobenzyl)oxy]-4-pyrimidinyl]-1,3-benzothiazol-2-
             1112979-60-8P, N-[6-[2-[(1,3-Benzodioxol-5-v1)methoxv]-4-
vllacetamide
pyrimidinyl]-1,3-benzothiazol-2-yl]acetamide
                                             1112979-61-9P.
N-[6-[2-[(3-Methoxyphenyl)sulfanyl]-4-pyrimidinyl]-1,3-benzothiazol-2-
vl]acetamide
              1112979-62-0P, N-[6-[2-(2,2-Dimethylpropoxy)-4-pyrimidinyl]-
                                 1112979-63-1P,
1,3-benzothiazol-2-vllacetamide
N-[6-[2-[((1R)-1-Phenylethyl)oxy]-4-pyrimidinyl]-1.3-benzothiazol-2-
yl]acetamide 1112979-64-2P, N-[6-[2-[3-(4-Pyridinyl)propoxy]-4-
pyrimidinyl]-1,3-benzothiazol-2-yl]acetamide 1112979-65-3P,
6-[2-[(3-Phenylpropyl)amino]-4-pyrimidinyl]-1,3-benzothiazol-2-amine
1112979-66-4P, N-[6-[2-[(3-Methoxypropy1)amino]-4-pyrimidiny1]-1,3-
benzothiazo1-2-y1]acetamide 1112979-67-5P,
N-[6-[2-[(2-Methoxyethyl)amino]-4-pyrimidinyl]-1,3-benzothiazol-2-
yl]acetamide 1112979-69-7P, 6-[2-[(2-Methoxyethyl)amino]-4-pyrimidinyl]-
1,3-benzothiazo1-2-amine 1112979-70-0P,
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N-[6-[2-[(Benzyl)amino]-4-pyrimidinyl]-1,3-benzothiazol-2-yl]acetamide
1112979-71-1P, N-[6-[2-(Methylsulfanyl)-4-pyrimidinyl]-1,3-benzothiazol-2-
              1112979-72-2P, N-[6-(2-Methoxy-4-pyrimidiny1)-1,3-
vl]acetamide
benzothiazol-2-vllacetamide 1112979-73-3P,
N-[6-[2-(Dimethylamino)-4-pyrimidinyl]-1.3-benzothiazo1-2-yl]acetamide
1112979-74-4P, N-[6-(2-Hydroxy-4-pyrimidiny1)-1,3-benzothiazol-2-
             1112979-75-5P, N-[6-[2-[(Benzyl)oxy]-4-pyrimidinyl]-1,3-
vllacetamide
benzothiazol-2-v1]-2-(4-morpholinyl)acetamide
                                              1112979-76-6P,
N-[6-[2-[(Benzyl)oxyl-4-pyrimidinyl]-1,3-benzothiazol-2-yl]-2-hydroxy-2-
methylpropanamide
                  1112979-77-7P.
N = [6 - [2 - [(Benzyl)oxy] - 4 - pyrimidinyl] - 1, 3 - benzothiazol - 2 - yl] - N' - methylurea
1112979-78-8P, N-[6-[2-[(Benzyl)oxy]-4-pyrimidinyl]-1,3-benzothiazol-2-
yl]propanamide 1112979-79-9P, N-[6-[2-[(Benzyl)oxy]-4-pyrimidinyl]-1,3-
benzothiazol-2-yl]benzamide
                            1112979-80-2P,
N-[6-[2-[(Benzy1)oxy]-4-pyrimidiny1]-1,3-benzothiazol-2-y1]-N',N'-
                    1112979-81-3P.
dimethylglycinamide
N-[6-[2-[(4-Methoxyphenyl)sulfonyl]-1,3-thiazol-5-yl]-1,3-benzothiazol-2-
yl]acetamide 1112979-82-4P, N-[6-[2-[(4-Methoxyphenyl)sulfanyl]-1,3-
thiazol-5-yl]-1,3-benzothiazol-2-yl]acetamide 1112979-83-5P,
N-[6-[2-[(2-Fluorophenyl)sulfonyl]-1,3-thiazol-4-yl]-1,3-benzothiazol-2-
yl]acetamide 1112979-84-6P, N-[6-[2-(Phenylsulfonyl)-1,3-thiazol-4-yl]-
1,3-benzothiazol-2-vllacetamide
                                1112979-85-7P,
N-[6-[6-(Phenylsulfonyl)-2-pyridinyl]-1,3-benzothiazol-2-yl]acetamide
1112979-86-8P, N-[6-[6-[(4-Fluorophenyl)sulfonyl]-2-pyridinyl]-1,3-
benzothiazol-2-yl]acetamide 1112979-88-0P,
N-[6-[6-[(3-Fluorophenyl)sulfonyl]-2-pyridinyl]-1,3-benzothiazol-2-
             1112979-89-1P, N-[6-[6-](4-Methoxyphenyl)sulfonyl]-2-
vllacetamide
                                           1112979-90-4P,
pvridinvl]-1,3-benzothiazol-2-vl]acetamide
N-[6-[6-[(3-Methoxyphenyl)sulfonyl]-2-pyridinyl]-1,3-benzothiazol-2-
yl]acetamide 1112979-91-5P, N-[6-[6-[(2-Methoxyphenyl)sulfonyl]-2-
pyridinyl]-1,3-benzothiazol-2-yl]acetamide
                                            1112979-92-6P,
N-[6-(2-Amino-1,3-benzothiazol-6-yl)-2-pyridinyl]benzenesulfonamide
1112979-93-7P, N-[6-(2-Amino-1,3-benzothiazol-6-v1)-2-pyridinyl]-2-
fluorobenzenesulfonamide
                         1112979-94-8P,
N-[6-[6-[6-[(2-Fluorophenyl)sulfonyl]amino]-2-pyridinyl]-1,3-benzothiazol-2-
vllacetamide
              1112979-95-9P, N-[6-[6-[Methyl](4-
methylphenyl)sulfonyl]amino]-2-pyridinyl]-1,3-benzothiazol-2-yl]acetamide
1112979-96-0P, N-[6-[6-[Methyl(phenylsulfonyl)amino]-2-pyridinyl]-1,3-
benzothiazol-2-yl]acetamide
                             1112979-97-1P,
N-[6-[2-[(Phenylsulfonyl)amino]-4-pyrimidinyl]-1,3-benzothiazol-2-
vllacetamide
              1112979-98-2P, N-[6-[2-[[(4-Methoxyphenyl)sulfonyl]amino]-4-
pyrimidinyl]-1,3-benzothiazol-2-yl]acetamide
                                             1112979-99-3P.
N-[6-[2-[[(3-Pyridinyl)sulfonyl]amino]-4-pyrimidinyl]-1,3-benzothiazol-2-
              1112980-00-3P, N-[6-[2-[[(4-Fluorophenyl)sulfonyl]amino]-4-
yl]acetamide
pyrimidinyl]-1,3-benzothiazol-2-yl]acetamide
                                              1112980-01-4P,
N-[6-[2-[](2-Fluorophenyl)sulfonyl]amino]-4-pyrimidinyl]-1,3-benzothiazol-
               1112980-02-5P, N-[6-[2-[[(3-Fluorophenvl)sulfonvl]amino]-
2-y1]acetamide
4-pyrimidinyl]-1,3-benzothiazol-2-yl]acetamide 1112980-03-6P,
N-[6-[2-[[(4-Methylphenyl)sulfonyl]amino]-4-pyrimidinyl]-1,3-benzothiazol-
                1112980-04-7P, N-[6-[2-[[(4-Ethylphenyl)sulfonyl]amino]-4-
2-vllacetamide
pyrimidinyl]-1,3-benzothiazol-2-yl]acetamide 1112980-05-8P,
N-[6-[2-[](3-Methoxyphenyl)sulfonyl]amino[-4-pyrimidinyl]-1,3-benzothiazol-
                1112980-06-9P, N-[4-[4-[2-(Acetylamino)-1,3-benzothiazol-
2-vllacetamide
6-v11-2-pvrimidinvl|sulfamovl|phenvl|acetamide
                                                1112980-07-0P.
N-[6-[2-[[(3,4-Dimethoxyphenyl)sulfonyl]amino]-4-pyrimidinyl]-1,3-
benzothiazol-2-yl]acetamide
                             1112980-08-1P,
N-[6-[2-[[(4-Methoxyphenyl)sulfonyl](methyl)amino]-4-pyrimidinyl]-1,3-
benzothiazo1-2-vl]acetamide 1112980-09-2P,
N-[6-[2-[Ethy1[(4-methoxypheny1)sulfony1]amino]-4-pyrimidiny1]-1,3-
benzothiazol-2-yl]acetamide 1112980-10-5P,
N-[6-[2-[Methyl[(4-methylphenyl)sulfonyl]amino]-4-pyrimidinyl]-1,3-
benzothiazo1-2-y1]acetamide 1112980-11-6P,
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N-[6-[2-[Methyl(phenylsulfonyl)amino]-4-pyrimidinyl]-1,3-benzothiazol-2-
              1112980-13-8P, N-[6-[2-[[(2-
vl]acetamide
Fluorophenyl)sulfonyl|(methyl)amino|-4-pyrimidinyl|-1,3-benzothiazol-2-
yl]acetamide
             1112980-14-9P, N-[6-[2-[Methv1](3-
methylphenyl)sulfonyllaminol-4-pyrimidinyll-1,3-benzothiazol-2-
yl]acetamide 1112980-15-0P, N-[7-(3-Fluoro-4-methoxyphenyl)-1,3-
benzothiazol-2-yl]acetamide 1112980-16-1P,
N-[7-(4-Methoxyphenyl)-1,3-benzothiazol-2-yl]acetamide
                                                        1112980-17-2P,
N-[7-(3-Methoxyphenyl)-1,3-benzothiazol-2-vl]acetamide 1112980-18-3P,
N-[6-[2-[(4-Fluorophenyl)sulfonyl]-1,3-thiazol-4-yl]-1,3-benzothiazol-2-
vllacetamide
             1112980-19-4P, N-[6-(2-0xo-2,3-Dihydrobenzo[d]thiazol-4-yl)-
1,3-benzothiazol-2-yl]acetamide 1112980-20-7P,
N-[6-(1H-Indazol-4-yl)-1,3-benzothiazol-2-yl]acetamide
                                                       1112980-21-8P,
N-[6-[2-[(1-Methyl-1-phenylethyl)amino]-4-pyrimidinyl]-1,3-benzothiazol-2-
yl]acetamide 1112980-22-9P, N-[6-(2-Amino-6-methyl-4-pyrimidinyl)-1,3-
benzothiazol-2-yl]acetamide
                            1112980-23-0P,
N-[6-[2-(3-Hydroxypropoxy)-4-pyrimidinyl]-1,3-benzothiazo1-2-yl]acetamide
1112980-24-1P, N-[6-[2-(4-Hydroxybutoxy)-4-pyrimidinyl]-1,3-benzothiazol-2-
             1112980-25-2P, N-[6-[2-(2-Hydroxyethoxy)-4-pyrimidinyl]-1,3-
yl]acetamide
benzothiazol-2-vl]acetamide
                            1112980-27-4P,
N-[6-[2-[(4-Methylbenzyl)oxy]-4-pyrimidinyl]-1,3-benzothiazol-2-
vllacetamide
             1112980-28-5P, N-[6-[2-[(3-Methylbenzyl)oxy]-4-pyrimidinyl]-
1,3-benzothiazol-2-vllacetamide
                                1112980-29-6P,
N-[6-[2-[(3-Methoxybenzyl)oxy]-4-pyrimidinyl]-1,3-benzothiazol-2-
             1112980-30-9P, N-[6-[2-[(3-Fluorophenyl)sulfanyl]-4-
vllacetamide
pyrimidinyl]-1,3-benzothiazol-2-yl]acetamide
                                             1112980-31-0P,
N-[6-[6-Methyl-5-[(phenylsulfonyl)amino]-3-pyridinyl]-1,3-benzothiazol-2-
              1112980-32-1P, N-[6-[5-[[(4-Fluorophenv1)sulfonv1]amino]-6-
vllacetamide
methyl-3-pyridinyl]-1,3-benzothiazol-2-yl]acetamide
                                                    1112980-34-3P.
N-[6-[5-[](2-Fluorophenyl)sulfonyl]amino]-6-methyl-3-pyridinyl]-1,3-
benzothiazo1-2-y1]acetamide
                            1112980-35-4P.
N-[6-[6-Methyl-5-[[[3-(trifluoromethyl)phenyl]sulfonyl]amino]-3-pyridinyl]-
1,3-benzothiazol-2-v1]acetamide
                                1112980-36-5P,
N-[6-[5-[[(4-tert-Butylphenyl)sulfonyl]amino]-6-methyl-3-pyridinyl]-1,3-
benzothiazol-2-vllacetamide
                            1112980-37-6P,
N-[6-[5-[[[3-(Difluoromethoxy)phenyl]sulfonyl]amino]-6-methyl-3-pyridinyl]-
1,3-benzothiazol-2-yl]acetamide
                                1112980-38-7P,
N-[6-[5-[[(4-Methoxyphenyl)sulfonyl]amino]-6-methyl-3-pyridinyl]-1,3-
benzothiazol-2-yl]acetamide
                             1112980-39-8P,
N-[4-Fluoro-6-[5-[[[4-(trifluoromethyl)phenyl]sulfonyl]amino]-3-pyridinyl]-
1,3-benzothiazol-2-vllacetamide
                                 1112980-40-1P,
N-[6-[6-[((4-Methoxyphenyl)sulfonyl]amino]-2-pyrazinyl]-1,3-benzothiazol-2-
yl]acetamide
              1112980-41-2P, N-[6-[5-[[(4-Acetylphenyl)sulfonyl]amino]-6-
chloro-3-pyridinyl]-1,3-benzothiazol-2-yl]acetamide
                                                    1112980-42-3P,
N-[6-[6-[(4-Methoxyphenyl)sulfonyl]-2-pyrazinyl]-1,3-benzothiazol-2-
vl]acetamide
              1112980-43-4P, N-[6-[6-[(2-Fluorophenv1)sulfonv1]-2-
pvrazinvl]-1,3-benzothiazol-2-vl]acetamide
                                           1112980-44-5P,
N-[6-[2-[(2,4-Dimethylphenyl)sulfanyl]-4-pyrimidinyl]-1,3-benzothiazol-2-
              1112980-45-6P, N-[6-[2-[(2,5-Dimethylphenyl)sulfanyl]-4-
vllacetamide
pyrimidinyl]-1,3-benzothiazol-2-yl]acetamide
                                             1112980-46-7P,
N-[6-[5-(Dimethylamino)-6-methoxy-3-pyridinyl]-1,3-benzothiazol-2-
vl]acetamide
              1112980-47-8P, N-[6-[2-[(2-Chlorophenyl)sulfanyl]-4-
pyrimidinyl]-1,3-benzothiazol-2-yl]acetamide
                                              1112980-48-9P,
N-[6-[6-[((4-Methoxyphenyl)sulfonyl](methyl)aminol-2-pyrazinyl]-1,3-
benzothiazol-2-yl]acetamide 1112980-49-0P,
N-[6-[6-[Methyl](4-methylphenyl)sulfonyl]amino]-2-pyrazinyl]-1,3-
benzothiazol-2-yl]acetamide
                             1112980-50-3P,
N-[6-[2-[(3,4-Dimethylphenyl)sulfanyl]-4-pyrimidinyl]-1,3-benzothiazol-2-
yl]acetamide 1112980-51-4P, N-[6-[2-[(2,6-Dimethylphenyl)sulfanyl]-4-
pyrimidinyl]-1,3-benzothiazol-2-yl]acetamide
                                             1112980-53-6P.
N-[6-[6-[(2-Fluorophenyl)sulfanyl]-2-pyrazinyl]-1,3-benzothiazol-2-
yl]acetamide 1112980-54-7P, N-[4-Fluoro-6-[2-[[(4-
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methoxyphenyl)sulfonyl]amino]-4-pyrimidinyl]-1,3-benzothiazol-2-
              1112980-56-9P, N-[6-[6-[(4-Methoxyphenyl)sulfanyl]-2-
vl]acetamide
pvrazinv1]-1,3-benzothiazo1-2-v1]acetamide
                                            1112980-57-0P,
N-[6-[2-[(2-Bromophenv1)sulfanv1]-4-pvrimidinv1]-1,3-benzothiazol-2-
              1112980-58-1P.
vllacetamide
N-[6-[6-[(Benzyl)oxy]-2-pyrazinyl]-1,3-benzothiazol-2-yl]acetamide
1112980-59-2P, N-[5-[3-[[(4-Methylphenyl)sulfonyl]amino]phenyl]-
[1,3]thiazolo[5,4-b]pyridin-2-yl]acetamide
                                           1112980-60-5P,
N-[4-Fluoro-6-[6-[(2-fluorophenyl)sulfonyl]-2-pyridinyl]-1,3-benzothiazol-
2-vl]acetamide 1112980-61-6P, N-[6-[2-[(4-Chlorophenvl)sulfanvl]-4-
pyrimidinyll-1,3-benzothiazol-2-vllacetamide 1112980-62-7P.
N-[6-[2-[(4-Bromophenyl)sulfanyl]-4-pyrimidinyl]-1,3-benzothiazol-2-
vl]acetamide 1112980-63-8P, N-[6-[2-[(3-Chlorophenyl)sulfanyl]-4-
pyrimidinyl]-1,3-benzothiazol-2-vl]acetamide
                                             1112980-64-9P,
N-[6-[6-Chloro-5-[(1-methylethyl)amino]-3-pyridinyl]-1,3-benzothiazol-2-
yl]-2-(2-pyridinyl)acetamide 1112980-66-1P,
N-[4-Fluoro-6-[2-[[(4-methoxyphenyl)sulfonyl](methyl)amino]-4-pyrimidinyl]-
1,3-benzothiazol-2-yl]acetamide
                                 1112980-67-2P,
N-[6-[6-Chloro-5-[(1-methylethyl)amino]-3-pyridinyl]-1,3-benzothiazol-2-
yl]-2-methoxyacetamide
                        1112980-68-3P,
\tilde{N}-[6-[6-Methoxy-5-[(1-methylethyl)amino]-3-pyridinyl]-1,3-benzothiazol-2-
vllacetamide
              1112980-69-4P, N-[5-[3-[[(4-
Methoxyphenyl)sulfonyl]amino|phenyl]-[1,3]thiazolo[5,4-b]pyridin-2-
yl]acetamide
              1112980-70-7P, N-[6-[6-(Methylamino)-5-[(1-
methylethyl)amino]-3-pyridinyl]-1,3-benzothiazo1-2-vl]acetamide
1112980-71-8P, N-[4-Fluoro-6-[6-[(4-methoxyphenyl)sulfonyl]-2-pyridinyl]-
1.3-benzothiazol-2-v1]acetamide
                                1112980-72-9P,
N-[6-[2-[(3,5-Dimethylphenyl)sulfanyl]-4-pyrimidinyl]-1,3-benzothiazol-2-
vllacetamide
             1112980-74-1P, N-[6-[6-Chloro-5-[(1-methylethyl)amino]-3-
pyridinyl]-1,3-benzothiazol-2-yl]-2-((2S)-tetrahydro-2-furanyl)acetamide
1112980-75-2P, N-[6-[5-Amino-6-(methylamino)-3-pyridinyl]-1,3-benzothiazol-
2-yl]acetamide
                1112980-76-3P, N-[6-[6-[3-(Dimethylamino)propoxy]-5-[(1-
methylethyl)amino]-3-pyridinyl]-1,3-benzothiazol-2-yl]acetamide
1112980-77-4P, N-[6-[2-[(2-(1-Methylethyl)phenyl]sulfanyl]-4-pyrimidinyl]-
                                1112980-78-5P,
1,3-benzothiazol-2-vllacetamide
6-[6-Chloro-5-[(1-methylethyl)amino]-3-pyridinyl]-1,3-benzothiazol-2-amine
1112980-80-9P, N-[6-(2,2,3-Trimethyl-2,3-dihydro-1H-imidazo[4,5-b]pyridin-
6-yl)-1,3-benzothiazol-2-yl]acetamide 1112980-81-0P,
N-[6-[2-[(2,5-Dimethoxyphenyl)sulfanyl]-4-pyrimidinyl]-1,3-benzothiazol-2-
              1112980-83-2P, N-[6-[6-[2-(Dimethylamino)ethoxy]-5-[(1-
vl]acetamide
methylethyl)aminol-3-pyridinyll-1,3-benzothiazol-2-yllacetamide
1112980-84-3P, N-[6-[2-(4-Morpholinyl)-4-pyrimidinyl]-1,3-benzothiazol-2-
vllacetamide
              1112980-85-4P, N-[6-[6-Chloro-5-[[4-(1-hydroxy-1-
methylethyl)phenyl]sulfonyl]amino]-3-pyridinyl]-1,3-benzothiazol-2-
yl]acetamide
              1112980-86-5P, N-[6-[6-Chloro-5-[[(4-
fluorophenyl)sulfonyl]amino]-3-pyridinyl]-1,3-benzothiazo1-2-yl]acetamide
1112980-87-6P, N-[6-[6-Chloro-5-[[(4-methoxyphenyl)sulfonyl]amino]-3-
pyridinyl]-1,3-benzothiazol-2-vl]acetamide 1112980-88-7P.
N-[6-[5-[[(4-Fluorophenyl)sulfonyl]amino]-1,3,4-oxadiazol-2-yl]-1,3-
benzothiazol-2-yl]acetamide
                             1112980-89-8P.
N-[5-(2-Amino-1,3-benzothiazol-6-yl)-1,3,4-oxadiazol-2-yl]-4-
methylbenzenesulfonamide
                          1112980-91-2P, tert-Butyl
[6-[5-[[(4-fluorophenyl)sulfonyl]amino]-1,3,4-oxadiazol-2-yl]-1,3-
benzothiazol-2-vllcarbamate
                             1112980-95-6P, tert-Butyl
[6-[5-[(benzyl)(methylsulfonyl)amino]-1,3,4-oxadiazol-2-yl]-1,3-
benzothiazo1-2-y1]carbamate
                             1112980-96-7P.
N-[6-[6-Chloro-5-[(cyclohexylsulfonyl)amino]-3-pyridinyl]-1,3-benzothiazol-
2-v1]acetamide
                1112980-97-8P, N-[6-[6-Chloro-5-[[[3-
(trifluoromethyl)phenyl]sulfonyl]amino]-3-pyridinyl]-1,3-benzothiazol-2-
yl]acetamide 1112980-98-9P, N-[6-[5-[[(3-tert-
Butylphenyl)sulfonyl]amino]-6-chloro-3-pyridinyl]-1,3-benzothiazol-2-
yl]acetamide 1112980-99-0P, N-[6-[6-Chloro-5-[[(4-
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hydroxyphenyl)sulfonyl]amino]-3-pyridinyl]-1,3-benzothiazol-2-yl]acetamide
 1112981-00-6P, N-[6-[6-Chloro-5-[[(3,5-dichlorophenyl)sulfonyl]amino]-3-
 pyridiny1]-1,3-benzothiazo1-2-v1]acetamide 1112981-01-7P,
 N-[6-[6-Chloro-5-[[(3,5-difluorophenyl)sulfonyl]amino]-3-pyridinyl]-1,3-
 benzothiazo1-2-v1lacetamide
                              1112981-02-8P.
 N-[6-[6-Chloro-5-[(propylsulfonyl)amino]-3-pyridinyl]-1,3-benzothiazol-2-
               1112981-03-9P, N-[6-[5-[(Butylsulfonyl)amino]-6-chloro-3-
 vllacetamide
 pyridiny1]-1,3-benzothiazo1-2-y1]acetamide 1112981-04-0P,
 N-[6-[6-Chloro-5-[[(1-methylethyl)sulfonyl]amino]-3-pyridinyl]-1,3-
 benzothiazol-2-vllacetamide 1112981-06-2P,
 N-[6-[6-Chloro-5-[[(4-chlorophenyl)sulfonyl]amino]-3-pyridinyl]-1,3-
 benzothiazol-2-vllacetamide
                              1112981-07-3P.
 N-[6-[6-Chloro-5-[(phenylsulfonyl)amino]-3-pyridinyl]-1,3-benzothiazol-2-
 vl]acetamide
                1112981-08-4P, N-[6-[6-Chloro-5-[]]4-
 (difluoromethoxy)phenyl]sulfonyl]amino]-3-pyridinyl]-1,3-benzothiazol-2-
 yl]acetamide 1112981-09-5P, N-[6-[6-Chloro-5-[[(3-
 fluorophenyl)sulfonyl]amino]-3-pyridinyl]-1,3-benzothiazol-2-yl]acetamide
 1112981-10-8P, N-[6-[6-Chloro-5-[[[3-
  (difluoromethoxy)phenyl]sulfonyl]amino]-3-pyridinyl]-1,3-benzothiazol-2-
               1112981-11-9P, N-[6-[6-Chloro-5-[](3-
 vl]acetamide
 chlorophenyl)sulfonyl]amino]-3-pyridinyl]-1,3-benzothiazo1-2-yl]acetamide
1112981-12-0P, N-[6-[6-Chloro-5-[[(thiophen-2-v1)sulfonv1]amino]-3-
 pvridinvll-1,3-benzothiazol-2-vllacetamide 1112981-13-1P.
 N-[6-[6-Chloro-5-[(thiophen-3-v1)sulfonv1]amino]-3-pvridinv1]-1.3-
 benzothiazol-2-vllacetamide
                               1112981-14-2P.
 N-[6-[5-[(Benzylsulfonyl)amino]-6-chloro-3-pyridinyl]-1,3-benzothiazol-2-
                1112981-15-3P, N-[6-[6-Chloro-5-[[(4-
 vllacetamide
 methylphenyl)sulfonyl|amino|-3-pyridinyl|-1,3-benzothiazol-2-yl|acetamide
 1112981-16-4P, N-[6-[6-Chloro-5-[[]4-
 (trifluoromethyl)phenyl]sulfonyl]amino]-3-pyridinyl]-1,3-benzothiazol-2-
 yl]acetamide
                1112981-17-5P, N-[6-[5-[[(4-tert-
 Butylphenyl)sulfonyl]amino]-6-chloro-3-pyridinyl]-1,3-benzothiazol-2-
                1112981-18-6P, N-[5-(2-Amino-1,3-benzothiazol-6-v1)-2-
 vl]acetamide
                                                 1112981-19-7P,
 chloro-3-pvridinvll-4-fluorobenzenesulfonamide
 N-[6-[6-Chloro-5-[[(5-chlorothiophen-2-yl)sulfonyl]amino]-3-pyridinyl]-1,3-
 benzothiazol-2-vllacetamide
                              1112981-20-0P.
 N-[6-[5-[[(4-Methylphenyl)sulfonyl]amino]-3-pyridinyl]-1,3-benzothiazol-2-
 yl]acetamide
                1112981-22-2P, N-[6-[5-[[(4-Methoxyphenyl)sulfonyl]amino]-3-
 pyridinyl]-1,3-benzothiazol-2-yl]acetamide
                                              1112981-23-3P,
 N-[6-[5-[[[4-(Trifluoromethyl)phenyl]sulfonyl]amino]-3-pyridinyl]-1,3-
 benzothiazol-2-vllacetamide
                              1112981-24-4P,
 N-[6-[5-[[[3-(Trifluoromethyl)phenyl]sulfonyl]amino]-3-pyridinyl]-1,3-
 benzothiazol-2-vllacetamide
                              1112981-25-5P.
 N-[6-[5-[[(4-Fluorophenyl)sulfonyl]amino]-3-pyridinyl]-1,3-benzothiazol-2-
 vl]acetamide
               1112981-26-6P, N-[6-[5-[[(3-Fluorophenyl)sulfonyl]amino]-3-
 pyridinyl]-1,3-benzothiazol-2-vl]acetamide 1112981-27-7P,
 \tilde{N}-[6-[5-[[(3,4-Dichlorophenyl)sulfonyl]amino]-3-pyridinyl]-1,3-
 benzothiazol-2-vllacetamide
                               1112981-28-8P.
 N-[6-[5-[[(4-tert-Butylphenyl)sulfonyl]amino]-3-pyridinyl]-1.3-
 benzothiazol-2-vllacetamide
                               1112981-29-9P.
 N-[6-[5-[(Phenylsulfonyl)amino]-3-pyridinyl]-1,3-benzothiazol-2-
 vl]acetamide
                1112981-30-2P, N-[6-[2-[[(4-
 Fluorophenyl)sulfonyl](methyl)aminol-4-pyrimidinyl]-1,3-benzothiazol-2-
 vllacetamide
                1112981-31-3P, N-[6-[2-[Methyl](6-
 quinolinyl)sulfonyl]amino]-4-pyrimidinyl]-1,3-benzothiazol-2-yl]acetamide
 1112981-32-4P, N-[6-[2-[[(4-tert-Butylphenyl)sulfonyl](methyl)amino]-4-
 pyrimidinyl]-1,3-benzothiazol-2-yl]acetamide
                                                1112981-33-5P,
 N-[6-[2-[N-Methyl-N-[(thiophen-2-yl)sulfonyl]amino]-4-pyrimidinyl]-1,3-
 benzothiazo1-2-v1|acetamide 1112981-34-6P,
 N-[6-[2-[Methyl](1-naphthalenyl)sulfonyl]amino]-4-pyrimidinyl]-1,3-
 benzothiazol-2-yl]acetamide 1112981-35-7P,
 N-[6-[2-[[(5-Isoquinoliny1)sulfony1](methy1)amino]-4-pyrimidiny1]-1,3-
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benzothiazol-2-vllacetamide
                             1112981-36-8P,
N-[6-[2-[N-Methyl-N-[(thiophen-3-yl)sulfonyl]amino]-4-pyrimidinyl]-1,3-
                             1112981-37-9P,
benzothiazo1-2-v1|acetamide
N-[6-[2-[[(3,4-Dimethylphenyl)sulfonyl](methyl)amino]-4-pyrimidinyl]-1,3-
benzothiazol-2-v1lacetamide
                              1112981-38-0P.
N-[6-[2-[Methyl-](1-methyl-1H-imidazol-4-yl)sulfonyl]aminol-4-pvrimidinvl]-
1,3-benzothiazol-2-yl]acetamide
                                  1112981-39-1P.
N-[6-[2-[(2,4-Dimethylphenyl)sulfonyl](methyl)amino]-4-pyrimidinyl]-1,3-
benzothiazol-2-vllacetamide
                             1112981-40-4P,
N-[6-[2-[Methyl][4-(trifluoromethyl)phenyl]sulfonyl]amino]-4-pyrimidinyl]-
1,3-benzothiazol-2-yl]acetamide
                                 1112981-42-6P.
N-[6-[2-[Methyl[(2-naphthalenyl)sulfonyl]amino]-4-pyrimidinyl]-1,3-
benzothiazol-2-yl]acetamide
                             1112981-43-7P,
N-[6-[2-[Methyl](4-methylphenyl)sulfonyl]amino]-4-pyridinyl]-1,3-
benzothiazol-2-yl]acetamide
                             1112981-44-8P,
N-[6-[2-[[(4-Methylphenyl)sulfonyl]amino]-4-pyridinyl]-1,3-benzothiazol-2-
yl]acetamide 1112981-45-9P, N-[6-[2-[[(4-Methoxyphenyl)sulfonyl]amino]-4-
pyridinyl]-1,3-benzothiazol-2-yl]acetamide 1112981-46-0P,
N-[6-[5-[Methyl[[4-(trifluoromethyl)phenyl]sulfonyl]amino]-3-pyridinyl]-
1,3-benzothiazol-2-vl]acetamide
                                 1112981-47-1P,
N-[6-[5-[[(4-Fluorophenv1)sulfonv1](methv1)amino]-3-pvridinv1]-1,3-
benzothiazol-2-vllacetamide
                            1112981-48-2P.
N-[6-[5-[[(4-Chlorophenvl)sulfonvl](methvl)amino]-3-pvridinvl]-1,3-
benzothiazol-2-vllacetamide
                            1112981-49-3P.
N-[6-[5-[[(3,4-Dichlorophenyl)sulfonyl](methyl)amino]-3-pyridinyl]-1,3-
benzothiazol-2-vl]acetamide
                             1112981-50-6P,
N-[6-[5-[[(3,4-Difluorophenyl)sulfonyl](methyl)amino]-3-pyridinyl]-1,3-
benzothiazol-2-vllacetamide
                            1112981-51-7P,
N-[6-[5-[[(4-tert-Butylphenyl)sulfonyl](methyl)amino]-3-pyridinyl]-1.3-
benzothiazol-2-vllacetamide
                            1112981-52-8P.
N-[6-[5-[Methyl(phenylsulfonyl)amino]-3-pyridinyl]-1,3-benzothiazol-2-
              1112981-53-9P, N-[6-[6-[Methyl](3-
yl]acetamide
methylphenyl)sulfonyl]amino]-2-pyridinyl]-1,3-benzothiazo1-2-yl]acetamide
1112981-55-1P, N-[6-[6-[[(2-Fluorophenyl)sulfonyl](methyl)amino]-2-
pyridinyl]-1,3-benzothiazol-2-yl]acetamide
                                           1112981-56-2P,
N-[6-[6-(tert-Butylamino)-2-pyrazinyl]-1,3-benzothiazol-2-yl]acetamide
1112981-57-3P, N-[5-[5-[[(4-Fluorophenyl)sulfonyl]amino]-3-pyridinyl]-
[1,3]thiazolo[5,4-b]pyridin-2-yl]acetamide
                                            1112981-58-4P,
N-[6-[5-[2-(2-Oxo-1-pyrrolidinyl)ethoxy]-3-pyridinyl]-1,3-benzothiazol-2-
vl]acetamide
              1112981-59-5P,
N-[6-[5-[2-(4-Morpholinvl)ethoxv]-3-pvridinvl]-1,3-benzothiazol-2-
vllacetamide
              1112981-60-8P, N-[6-[5-[1-Methyl-2-(4-morpholinyl)ethoxyl-3-
pyridinyl]-1,3-benzothiazol-2-vl]acetamide
                                            1112981-61-9P.
N-[6-[5-[2-(2-0xo-1,3-oxazolidin-3-y1)]] ethoxy]-3-pyridiny1]-1,3-
benzothiazol-2-v1]acetamide
                             1112981-62-0P,
N-[6-[5-[2-(1-Piperidinyl)ethoxy]-3-pyridinyl]-1,3-benzothiazol-2-
yl]acetamide
              1112981-63-1P, N-[6-[5-[2-(1-Azepanvl)ethoxy]-3-pyridinvl]-
                                 1112981-64-2P.
1,3-benzothiazol-2-vllacetamide
N-[6-[6-Chloro-5-(tetrahydro-3-furanyloxy)-3-pyridinyl]-1,3-benzothiazol-2-
               1112981-65-3P, N-[6-[6-Chloro-5-(1-methylethoxy)-3-
vllacetamide
pyridinyl]-1,3-benzothiazol-2-yl]acetamide
                                            1112981-66-4P,
N-[6-[6-Chloro-5-[((3S)-tetrahydrofuran-3-yl)oxy]-3-pyridinyl]-1,3-
benzothiazol-2-vllacetamide
                             1112981-67-5P,
N-[6-(6-Bromo-5-methoxy-3-pyridinyl)-1,3-benzothiazol-2-yl]acetamide
1112981-69-7P, N-[6-(6-Chloro-5-fluoro-3-pyridiny1)-1,3-benzothiazol-2-
vllacetamide
              1112981-70-0P, N-[6-(6-Chloro-5-ethoxy-3-pyridiny1)-1,3-
benzothiazol-2-yl]acetamide 1112981-71-1P,
N-[6-(6-Chloro-5-methoxy-3-pyridinyl)-1,3-benzothiazo1-2-yl]acetamide
1112981-72-2P, N-[6-(4-Methoxy-3-pyridiny1)-1,3-benzothiazo1-2-
yl]acetamide 1112981-73-3P, N-[6-(6-Methoxy-3-pyridinyl)-1,3-
benzothiazo1-2-y1]acetamide 1112981-74-4P,
N-[6-(6-Ethoxy-3-pyridiny1)-1,3-benzothiazol-2-y1]acetamide
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RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of 2-aminobenzothiazole derivs. as PI3 kinase modulators) 112981-75-5P, N-[6-(6-Methoxy-4-methyl-3-pyridinyl)-1,3-benzothiazol-2-
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1112981-75-5P, N-[6-(6-Methoxy-4-methyl-3-pyridinyl)-1,3-benzothiazol-2-
yl]acetamide
              1112981-76-6P, N-[6-(4-Methyl-3-pyridinyl)-1,3-benzothiazol-
                1112981-77-7P, N-[6-(6-Chloro-4-methoxy-3-pyridinyl)-1,3-
2-vllacetamide
benzothiazol-2-vl[acetamide 1112981-78-8P,
N-[6-[6-Chloro-5-(difluoromethoxy)-3-pyridinyl]-1,3-benzothiazol-2-
vllacetamide
             1112981-79-9P, N-[6-[4-(Difluoromethoxy)-3-pyridinyl]-1,3-
benzothiazol-2-vllacetamide 1112981-80-2P,
N-[6-[6-(Difluoromethoxy)-3-pyridinyl]-1,3-benzothiazol-2-yl]acetamide
1112981-81-3P, N-[6-[6-(Difluoromethoxy)-4-methyl-3-pyridinyl]-1,3-
benzothiazol-2-vl|acetamide
                            1112981-82-4P,
N-[6-[4-(Hydroxymethyl)-3-pyridinyl]-1,3-benzothiazol-2-yl]acetamide
1112981-83-5P, N-[6-[5-[2-(3,3-Dimethyl-2-oxo-1-pyrrolidinyl)ethoxy]-3-
pyridinyl]-1,3-benzothiazol-2-yl]acetamide 1112981-84-6P,
N-[6-[5-[2-(3-Methyl-2-oxo-1-pyrrolidinyl)ethoxy]-3-pyridinyl]-1,3-
benzothiazol-2-yl]acetamide
                            1112981-86-8P,
N-[6-[5-[2-(3,3]] - Diffluoro-2-oxo-1-pyrrolidiny]) ethoxy]-3-pyridiny]-1,3-
                            1112981-87-9P,
benzothiazol-2-vl|acetamide
N-[6-[5-[2-(3-Fluoro-2-oxo-1-pyrrolidinyl)ethoxy]-3-pyridinyl]-1,3-
benzothiazol-2-vllacetamide 1112981-88-0P,
N-[6-[6-Chloro-5-[[[4-(1-hydroxyethyl)phenyl]sulfonyl]amino[-3-pyridinyl]-
1.3-benzothiazol-2-vllacetamide 1112981-89-1P.
N-[6-[5-[[4-(1-Hydroxyethyl)phenyl]sulfonyl]amino]-3-pyridinyl]-1,3-
benzothiazol-2-vl[acetamide 1112981-90-4P,
N-[6-[3-[[(4-Methoxyphenyl)sulfonyl]amino]phenyl]-1,3-benzothiazol-2-
vllacetamide
             1112981-91-5P, N-[6-[2-[(Tetrahydro-2H-pyran-4-yl)amino]-4-
pyrimidinyl]-1,3-benzothiazol-2-yl]acetamide
                                              1112981-92-6P.
N-[6-[2-[(2R)-2-(2-Methylphenyl)-1-pyrrolidinyl]-4-pyrimidinyl]-1,3-
benzothiazol-2-yl]acetamide
                            1112981-93-7P,
N-[6-[2-(1-Piperidinyl)-4-pyrimidinyl]-1,3-benzothiazol-2-yl]acetamide
1112981-94-8P, N-[6-[2-[(2-Pyridinyl)amino]-4-pyrimidinyl]-1,3-
                             1112981-95-9P,
benzothiazol-2-vllacetamide
N-[6-[2-[(1-Piperidinyl)amino]-4-pyrimidinyl]-1,3-benzothiazol-2-
             1112981-96-0P, N-[6-[2-((2R)-2-Phenyl-1-pyrrolidinv1)-4-
pyrimidinyl]-1,3-benzothiazol-2-yl]acetamide
                                             1112981-97-1P,
N-[6-[6-Cyano-5-[[(4-methoxyphenyl)sulfonyl]amino]-3-pyridinyl]-1,3-
benzothiazol-2-vllacetamide
                             1112981-98-2P,
N-[6-(5-Amino-6-cvano-3-pvridinvl)-1,3-benzothiazol-2-vl]acetamide
1112982-00-9P, Phenyl [6-[6-chloro-5-(dimethylamino)-3-pyridinyl]-1,3-
benzothiazol-2-vllcarbamate
                             1112982-01-0P,
N-[6-[6-Chloro-5-(dimethylamino)-3-pyridinyl]-1,3-benzothiazol-2-yl]-2-
methoxyacetamide
                 1112982-02-1P, N-[6-[6-Chloro-5-(dimethylamino)-3-
pyridinyl]-1,3-benzothiazol-2-vl]-2-phenoxyacetamide
                                                     1112982-03-2P,
N-[6-[6-Chloro-5-(dimethylamino)-3-pyridinyl]-1,3-benzothiazol-2-yl]-N-[2-
(4-morpholinvl)ethvllurea
                          1112982-04-3P.
6-[6-Chloro-5-(dimethylamino)-3-pyridinyl]-1,3-benzothiazol-2-amine
1112982-05-4P, N-[6-[6-Chloro-5-(dimethylamino)-3-pyridinyl]-1,3-
benzothiazol-2-yl]-N', N'-dimethylglycinamide
                                             1112982-06-5P,
N-[6-[6-Chloro-5-(dimethylamino)-3-pyridinyl]-1,3-benzothiazol-2-
                      1112982-07-6P, tert-Butyl
vl]methanesulfonamide
N-(tert-butoxycarbonyl)-N-[5-[2-(acetylamino)-1,3-benzothiazol-6-yl]-2-
chloro-3-pyridinyl]carbamate
                             1112982-08-7P.
N-[6-[5-(Cyanomethoxy)-3-pyridiny1]-1,3-benzothiazo1-2-y1]acetamide
1112982-10-1P, N-[6-(5-Fluoro-3-pyridinyl)-1,3-benzothiazol-2-yl]acetamide
1112982-11-2P, N-[6-[6-Chloro-5-(1-cyanoethoxy)-3-pyridiny1]-1,3-
benzothiazo1-2-y1]acetamide 1112982-12-3P,
N-[6-[2-Chloro-5-(1-cyanoethoxy)-3-pyridinyl]-1,3-benzothiazol-2-
yl]acetamide 1112982-13-4P, N-[6-[6-Chloro-5-[(2-methoxyethoxy)methoxy]-
3-pyridiny1]-1,3-benzothiazo1-2-y1]acetamide 1112982-14-5P,
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N-[6-[5-[(2-Methoxyethoxy)methoxy]-6-(trifluoromethyl)-3-pyridinyl]-1,3-
benzothiazo1-2-v1|acetamide
                             1112982-15-6P,
N-[6-[5-[((2R)-5-0xo-2-pyrrolidiny])]] methoxy[-3-pyridinyl]-1,3-benzothiazol-
2-v1]acetamide 1112982-16-7P, N-[6-[5-[(1-Aminocyclopropyl)methoxyl-3-
pyridinyl]-1,3-benzothiazol-2-yl]acetamide 1112982-17-8P,
N-[6-(5-Hydroxy-3-pyridinyl)-1,3-benzothiazol-2-yl]acetamide
1112982-18-9P, N-[6-(6-Chloro-3-pyridinyl)-1,3-benzothiazol-2-yl]acetamide
1112982-19-0P, N-[2-[[5-[2-(Acetylamino)-1,3-benzothiazol-6-y1]-3-
pvridinvl|oxv|ethvl|-2-methoxvacetamide 1112982-20-3P,
N-[6-[6-(3-Azabicvclo[3.2.2]nonan-3-yl)-2-pyrazinyl]-1,3-benzothiazol-2-
yl]acetamide 1112982-21-4P, N-[6-(6-Chloro-5-hydroxy-3-pyridinyl)-1,3-
benzothiazol-2-yl]acetamide 1112982-22-5P,
N-[6-[5-Hydroxy-6-(trifluoromethyl)-3-pyridinyl]-1,3-benzothiazol-2-
              1112982-24-7P, 5-[2-(Acetylamino)-1,3-benzothiazol-6-y1]-2-
vl]acetamide
chloropyridin-3-vl acetate 1112982-25-8P,
N-[6-[6-Chloro-5-[(4-methoxyphenyl)sulfonyl]amino]-3-pyridinyl]-1,3-
benzothiazol-2-yl]cyclohexanecarboxamide 1112982-26-9P,
N-[2-Chloro-5-[2-[(1-methylethyl)amino]-1,3-benzothiazol-6-yl]-3-
pyridinyl]-4-methoxybenzenesulfonamide 1112982-27-0P,
N-[2-Chloro-5-[2-[(cyclohexylmethyl)amino]-1,3-benzothiazol-6-yl]-3-
pyridinyl | -4-methoxybenzenesulfonamide 1112982-28-1P,
N-[5-(2-Amino-1,3-benzothiazol-6-v1)-2-chloro-3-pvridinv1]-3-
(difluoromethoxy)benzenesulfonamide
                                    1112982-29-2P,
N-[5-(2-Amino-1.3-benzothiazol-6-v1)-2-chloro-3-pyridinyl]-2-chloro-4-
(trifluoromethyl)benzenesulfonamide 1112982-30-5P.
N-[5-(2-Amino-1,3-benzothiazol-6-yl)-2-chloro-3-pyridinyl]-2-chloro-4-
fluorobenzenesulfonamide 1112982-31-6P,
N-[5-(2-Amino-1,3-benzothiazol-6-v1)-2-chloro-3-pyridinv1]-2,4-
dichlorobenzenesulfonamide 1112982-32-7P.
N-[5-(2-Amino-1,3-benzothiazol-6-v1)-2-chloro-3-pyridiny1]-2,4-
difluorobenzenesulfonamide 1112982-33-8P,
N-[5-(2-Amino-1,3-benzothiazol-6-yl)-2-chloro-3-pyridinyl]-4-fluoro-2-
methylbenzenesulfonamide 1112982-34-9P,
N-[5-(2-Amino-1,3-benzothiazol-6-v1)-2-chloro-3-pvridinvl]-4-chloro-2-
fluorobenzenesulfonamide 1112982-35-0P.
N-[5-(2-Amino-1,3-benzothiazol-6-v1)-2-chloro-3-pyridinvl]-2-
(trifluoromethyl) benzenesulfonamide
                                    1112982-36-1P.
6-[5-(tert-Butylamino)-6-chloro-3-pyridinyl]-1,3-benzothiazol-2-amine
1112982-37-2P, N-[6-[6-Chloro-5-[[(1-piperidinyl)sulfonyl]amino]-3-
pyridinyl]-1,3-benzothiazol-2-vl]acetamide 1112982-38-3P,
N-[2-Chloro-5-[2-(methylamino)-1,3-benzothiazol-6-v1]-3-pvridinvl]-4-
fluorobenzenesulfonamide 1112982-39-4P.
2-Chloro-N-[2-chloro-5-[2-(methylamino)-1,3-benzothiazol-6-vl]-3-
pyridinyl]-6-methylbenzenesulfonamide 1112982-40-7P,
2,6-Dichloro-N-[2-chloro-5-[2-(methylamino)-1,3-benzothiazol-6-yl]-3-
pyridinyl|benzenesulfonamide
                             1112982-41-8P,
\tilde{N}-[2-Chloro-5-[2-(methylamino)-1,3-benzothiazol-6-vl]-3-pyridinyl]-2-
fluorobenzenesulfonamide 1112982-42-9P,
4-Acetyl-N-[2-chloro-5-[2-(methylamino)-1,3-benzothiazol-6-v1]-3-
pyridinyl|benzenesulfonamide
                             1112982-43-0P.
N-[1-[4-[(2-Chloro-5-[2-(methylamino)-1,3-benzothiazol-6-yl]-3-
pyridinyl|sulfamoyl|phenyl|-1-methylethyl|acetamide
                                                    1112982-44-1P,
N-[1-[4-[[5-(2-Amino-1,3-benzothiazol-6-y1)-2-chloro-3-
pyridinyl]sulfamoyl]phenyl]-1-methylethyl]acetamide
                                                     1112982-45-2P.
N-[5-(2-Amino-1,3-benzothiazol-6-yl)-2-chloro-3-pyridinyl]-4-(1-hydroxy-1-
methylethyl)benzenesulfonamide 1112982-46-3P,
4-Acetyl-N-[5-(2-amino-1,3-benzothiazol-6-yl)-2-chloro-3-
pyridinyl|benzenesulfonamide
                             1112982-47-4P,
N-[5-(1,3-Benzoxazol-6-v1)-2-chloro-3-pyridiny1]-4-
fluorobenzenesulfonamide 1112982-48-5P,
N-[2-Chloro-5-[2-(methylsulfanyl)-1,3-benzothiazol-6-yl]-3-pyridinyl]-4-
methoxybenzenesulfonamide 1112982-51-0P,
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1-[5-(1,3-Benzothiazol-6-yl)-3-pyridinyl]ethanone 1112982-52-1P,
6-Fluoro-5-(2-methyl-1,3-benzothiazol-6-yl)-2-(trifluoromethyl)-3-
           1112982-53-2P, N-[6-[6-Chloro-5-[[[4-((1S)-1-
pyridinol
hydroxyethyl)phenyl|sulfonyl|amino|-3-pyridinyl|-1,3-benzothiazol-2-
yl]acetamide
             1112982-54-3P, N-[6-[6-Chloro-5-[[[4-((1R)-1-
hydroxyethyl)phenyl|sulfonyl|amino|-3-pyridinyl|-1,3-benzothiazol-2-
yl]acetamide 1112982-55-4P, N-[6-[6-(2-Fluorophenylsulfonyl)pyridin-2-
vl]-1,3-benzothiazol-2-vl]acetamide 1112982-67-8P,
N-[6-(3-Fluoro-4-methoxyphenyl)-1,3-benzothiazol-2-yl]acetamide
1112982-96-3P, N-[5-[5-[](4-Fluorophenyl)sulfonyl]amino[pyridin-3-
vllthiazolo[5,4-b]pyridin-2-vllacetamide trifluoroacetate 1112982-99-6P.
N-[6-[2-[2-(o-Tolyl)pyrrolidin-1-yl]pyrimidin-4-yl]-1,3-benzothiazol-2-
yl]acetamide 1112983-00-2P, N-[6-[2-(2-Phenylpyrrolidin-1-yl)pyrimidin-4-
v1]-1,3-benzothiazol-2-v1]acetamide
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
(Uses)
   (preparation of 2-aminobenzothiazole derivs. as PI3 kinase modulators)
110-89-4, Piperidine, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
   (preparation of 2-aminobenzothiazole derivs. as PI3 kinase modulators)
1112980-26-3P, N-[6-(2-Chloro-4-pyrimidinyl)-1,3-benzothiazol-2-
yl]acetamide 1112980-73-0P, N-[6-(6-(6-Chloro-2-pyrazinyl)-1,3-benzothiazol-2-yl]acetamide 1112980-90-1P, tert-Butyl
[6-[5-[((4-methylphenyl)sulfonyl]amino]-1,3,4-oxadiazol-2-yl]-1,3-
benzothiazol-2-vl]carbamate 1112980-93-4P, tert-Butyl
[6-[5-[(benzyl)amino]-1,3,4-oxadiazol-2-yl]-1,3-benzothiazol-2-
yl]carbamate 1112981-99-3P, N-[6-[6-Chloro-5-(dimethylamino)-3-
pyridinyl]-1,3-benzothiazol-2-yl]acetamide
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic
preparation); THU (Therapeutic use); BIOL (Biological study); PREP
(Preparation); RACT (Reactant or reagent); USES (Uses)
   (reactant; preparation of 2-aminobenzothiazole derivs. as PI3 kinase
  modulators)
50-00-0, Formaldehyde, reactions 67-64-1, Acetone, reactions
                                                                70-55-3,
4-Methylbenzenesulfonamide 74-89-5, Methylamine, reactions 75-04-7,
Ethylamine, reactions 75-16-1, Methylmagnesium bromide
2-Propanamine, reactions 75-64-9, 2-Methylpropan-2-amine, reactions
98-09-9, Benzenesulfonyl chloride 98-10-2, Benzenesulfonamide
4-Methylbenzene-1-sulfonyl chloride
                                    98-60-2
                                              98-68-0
Cyclohexanecarboxylic acid 105-53-3, Diethyl malonate
2-Chloroacetonitrile 108-01-0, 2-(Dimethylamino)
ethanol 108-21-4, Isopropyl acetate 108-24-7, Acetic anhydride
124-63-0, Methanesulfonyl chloride 283-24-9, 3-Azabicyclo[3.2.2]nonane
349-88-2, 4-Fluorobenzenesulfonyl chloride 371-42-6,
4-Fluorobenzenethiol 407-20-5, 3-Bromo-5-fluoropyridine
                                                           504-29-0.
               585-32-0, Cumvlamine 592-84-7, n-Butvl formate
2-Pyridinamine
622-78-6, Benzyl isothiocyanate 640-61-9, N-Methyl-p-toluenesulfonamide
                                701-99-5
696-63-9, 4-Methoxybenzenethiol
                                            771-61-9.
2,3,4,5,6-Pentafluorophenol 925-90-6, Ethylmagnesium bromide
1006-64-0, 2-Phenylpyrrolidine 1118-68-9, 2-(Dimethylamino) acetic acid
1617-17-0, 2-Chloropropanenitrile 1885-14-9, Phenyl chloroformate
1899-93-0, m-Toluenesulfonvl chloride
                                       2038-03-1, 4-Morpholineethanamine
2038-57-5, 3-Phenylpropylamine 2213-43-6, 1-Piperidinamine
                                                              2290-65-5,
Trimethylsilyl isothiocyanate 2402-78-0, 2,6-Dichloropyridine
2557-78-0, 2-Fluorobenzenethiol 2859-67-8, 3-(Pyridin-3-y1)-1-propanol
2905-21-7 2991-42-6, 4-(Trifluoromethyl)benzene-1-sulfonyl chloride
3218-02-8, Cyclohexylmethanamine 3445-11-2,
1-(2-Hydroxyethyl)pyrrolidin-2-one 3934-20-1, 2,4-Dichloropyrimidine
3970-21-6, 2-Methoxyethoxymethyl chloride 4175-77-3, 2,4-Dibromothiazole
4837-38-1, Cyclohexanesulfonyl chloride 5600-21-5,
4-Chloro-6-methylpyrimidin-2-amine 5720-07-0, 4-Methoxyphenylboronic
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ΙT

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acid
     7087-68-5, N-Ethyl-N-isopropylpropan-2-amine 13250-46-9, Acetyl
               13535-01-8 16133-25-8, 3-Pyridinesulfonyl chloride
isothiocvanate
16179-97-8, 2-Pyridylacetic acid hydrochloride 19798-81-3,
6-Bromopyridin-2-amine 21327-14-0, N-(3-Bromophenyl)thiourea
30418-59-8, 3-Aminophenylboronic acid 31784-72-2,
N-(5-Chlorothiazolo[5,4-b]pyridin-2-y1)acetamide
                                                 38041-19-9.
4-Aminotetrahydro-2H-pyran 38870-89-2, 2-Methoxyacetyl chloride
38940-62-4 39856-57-0, 2,6-Dibromopyridin-3-amine
6-Chloropyridin-2-amine 55758-32-2, 2-Fluoro-5-hydroxypyridine
62673-31-8, Benzylzinc bromide 66673-40-3,
                                           67443-38-3,
(R)-(-)-5-(Hydroxymethyl)-2-pyrrolidinone
5-Bromo-2-chloro-3-nitropyridine 67567-26-4,
4-Bromo-2,6-difluorobenzenamine 68867-20-9,
6-Iodo-2-methylbenzo[d]thiazole 73183-34-3,
4,4,5,5-Tetramethyl-2-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-1,3,2-
dioxaborolane 73443-85-3, 4-Bromobenzo[d]thiazol-2(3H)-one 73583-37-6,
4-Bromo-2-chloropyridine 74115-13-2, 5-Bromopyridin-3-o1 80945-86-4,
6-Bromo-2-chlorobenzo[d]thiazole 129540-23-4, 2-(o-Tolyl)pyrrolidine
130115-85-4, 3-Bromo-2-chloropyridin-5-ol 149507-26-6,
3-Fluoro-4-methoxyphenylboronic acid
                                    153034-86-7,
2-Chloro-4-iodopyridine 175205-54-6,
2-Chloro-4-(trifluoromethyl)benzene-1-sulfonyl chloride 186407-74-9
225525-50-8, 2-(tert-Butoxycarbonylamino)-4-benzothiazole-6-carboxylic
     286946-77-8, 5-Bromo-2-chloropyridin-3-ol 351003-38-8,
3-(Difluoromethoxy) benzenesulfonyl chloride 375369-14-5,
6-Bromobenzo[d]oxazole 474966-97-7,
6-Bromo-2-(methylthio)-1,3-benzothiazole
                                         573675-27-1.
3-Amino-5-bromopicolinonitrile 588729-99-1,
5-Bromo-2-chloropyridin-3-amine 796061-08-0,
4-Methyl-N-[3-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-
yl)phenyl]benzenesulfonamide 887309-87-7,
N-(5-Bromo-2-chloropyridin-3-yl)-4-fluorobenzenesulfonamide
1112982-58-7, 5-Bromo-2-(4-methoxyphenylsulfonyl)thiazole
                                                          1112982-60-1,
2-Chloro-6-(4-fluorophenvlthio)pyridine 1112982-64-5,
N-[6-(4,4,5,5-Tetramethyl-1,3-dioxolan-2-yl)-1,3-benzothiazol-2-
yl]acetamide 1112982-78-1, 4-Acetyl-N-(5-bromo-2-chloropyridin-3-
yl) benzenesulfonamide 1112982-95-2,
(2-Acetamido-1,3-benzothiazol-6-yl)boronic acid
N-(5-Bromopyridin-3-yl)-4-(1-hydroxyethyl)benzenesulfonamide
1112982-98-5, N-[6-(3-Aminophenyl)-1,3-benzothiazol-2-yl]acetamide
1112983-01-3, N-(5-Bromo-2-cvanopyridin-3-v1)-4-methoxybenzenesulfonamide
1112983-04-6, tert-Butvl N-(tert-butoxycarbonvl)-N-(5-bromo-2-
chloropyridin-3-vl)carbamate
                             1112983-30-8.
N-(5-Bromo-2-chloropyridin-3-y1)-2-chloro-6-methylbenzenesulfonamide
1112983-32-0, N-[2-Chloro-5-(3,3,4,4-tetramethylborolan-1-yl)pyridin-3-yl]-
4-methoxybenzenesulfonamide
                            1113041-97-6
RL: RCT (Reactant); RACT (Reactant or reagent)
   (reactant; preparation of 2-aminobenzothiazole derivs, as PI3 kinase
  modulators)
ANSWER 2 OF 55 CAPLUS COPYRIGHT 2009 ACS on STN
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Entered STN: 15 Jan 2009
Use of a creatine-containing composition for improvement of memory
function including long-term memory and for prevention of mental fatigue.
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Gastner, Thomas; Selzer, Frauke; Krimmer, Hans-Peter; Hammer, Benedikt

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DN

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TN

SO

DT Patent LA German

PA

Alzchem Trostberg GmbH, Germany

Ger. Offen., 11pp. CODEN: GWXXBX CC 18-2 (Animal Nutrition)

Section cross-reference(s): 17, 63

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PATENT NO. KIND DATE APPLICATION NO. DATE

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CLASS

PATENT NO. CLASS PATENT FAMILY CLASSIFICATION CODES

DE 102007030495 IPCI A23L0001-30 [I,A]; A61K0031-198 [I,A]; A61K0031-185

[I,C*]; A61P0025-28 [N,A]; A61P0025-00 [N,C*] AB Described is the use of a solid or aqueous preparation containing creatine components

for improvement of memory function, memory retention, long-term memory and for preventing memory fatigue. The preparation contains at least one addnl. component from the group: Ginkgo biloba, ginseng, taiga root, yam root, lecithin, choline, phosphatidylserine, dimethylamino ethanol, acetylcholine, acetyl-L-carnitine, gluthathione, gluthathione, dimin a, vitamin A, vitamin E, vitamin Bl, vitamin B2, vitamin

glutamine, cysteine, vitamin A, vitamin E, vitamin B1, vitamin B2, vitam B6, vitamin B12, vitamin E, niacin, biotin, folic acid, pantothene acid, zinc, manganese, selenium, magnesium, coenzyme Q10, glucose, colostrum, synephrine, octopamine, caffeine, theophylline, a-linoleic acid, eicosapentaenoic acid, omega-3 fatty acids, piracetam, aniracetam, memantine, pyritinol, gallamine, vinpocetine and pangamic acid. The applied components behave here synergistically. Furthermore, the inventive prepns, have excellent organoleptic characteristics and a very

appried components behave here synergistically. Furthermore, the inventive prepns, have excellent organoleptic characteristics and a very high bioavailability. Due to these special advantages, the inventive prepns, are superbly suitable as food supplements, functional foods and animal feed additives.

ST brain function memory feed food additive nutraceutical creatine nutrient IT Natural products, pharmaceutical

Natural products, pharmaceutical (GinSeng; use of a creatine-containing composition for improvement of memory function including long-term memory and for prevention of mental fatigue)

IT Brain

(function of; use of a creatine-containing composition for improvement of

memory

function including long-term memory and for prevention of mental fatique)

IT Ginkgo biloba

(leaves; use of a creatine-containing composition for improvement of memory function including long-term memory and for prevention of mental fatique)

IT Memory, biological

(long-term, improvement of; use of a creatine-containing composition for improvement of memory function including long-term memory and for prevention of mental fatious)

T Fatigue, biological

(memory; use of a creatine-containing composition for improvement of memory function including long-term memory and for prevention of mental fatigue)

IT Acids, biological studies

RL: FFD (Food or feed use); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(organic; use of a creatine-containing composition for improvement of memory function including long-term memory and for prevention of mental fatique)

Fatty acids, biological studies

RL: FFD (Food or feed use); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(polyunsatd., omega-3; use of a creatine-containing composition for improvement

of memory function including long-term memory and for prevention of mental fatique)

IT Amnesia

(prevention of; use of a creatine-containing composition for improvement of memory function including long-term memory and for prevention of mental fatigue)

IT Acanthopanax senticosus

(root; use of a creatine-containing composition for improvement of memory function including long-term memory and for prevention of mental fatious)

IT Bioavailability Colostrum Dietary supplements Dioscorea Feed additives Flavor

> Food additives Food functional properties Fruit and vegetable juices Human

Memory, biological

Whey

Yam

(use of a creatine-containing composition for improvement of memory function including long-term memory and for prevention of mental fatigue) $\frac{1}{2}$

IT Amino acids, biological studies Bicarbonates

Carbohydrates, biological studies

Carbonydrates, biological studies Carbonates, biological studies Fats and Glyceridic oils, biological studies

Lecithins

Mineral elements, biological studies Phosphatidylserines

Proteins

Trace element nutrients

RL: FFD (Food or feed use); THU (Therapeutic use); BIOL (Biological

study); USES (Uses)
(use of a creatine-containing composition for improvement of memory function including long-term memory and for prevention of mental fatigue)

Milk preparations
(yogurt; use of a creatine-containing composition for improvement of memory
function including long-term memory and for prevention of mental
fatiume)

50-81-7D, Ascorbic acid, complexes and compds. with creatine Glucose, biological studies 51-84-3, Acetylcholine, biological studies 52-90-4, L-Cysteine, biological studies 56-84-8D, L-Aspartic acid, complexes and compds, with creatine 56-85-9, Glutamine, biological studies 57-00-1, Creatine 57-00-1D, Creatine, esters 58-08-2, Caffeine, biological studies 58-55-9, Theophylline, biological studies 58-85-5, Biotin 59-30-3, Folic acid, biological studies 59-43-8, Thiamin, biological studies 59-67-6, Niacin, biological studies 62-49-7, 59-67-6D, Nicotinic acid, complexes and compds. with creatine Choline 62-49-7D, Choline, complexes and compds. with creatine 63-68-3D, Methionine, complexes and compds. with creatine Formic acid, complexes and compds. with creatine 64-19-7D, Acetic acid, complexes and compds. with creatine 67-48-1, Choline chloride 68-19-9, Vitamin B12 70-18-8, Glutathione, biological studies 77-92-9D, Citric acid, complexes and compds. with creatine 79-83-4, Pantothenic acid 83-88-5, Riboflavin, biological studies 94-07-5, Synephrin 98-79-3D, Pyroglutamic acid, complexes and compds. with creatine 104-14-3, Octopamine 107-35-7D, Taurine, complexes and

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     Manganese, biological studies 7440-66-6, Zinc, biological studies
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     study); USES (Uses)
         (use of a creatine-containing composition for improvement of memory function
        including long-term memory and for prevention of mental fatigue)
RE.CNT 8
             THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD
(1) Anon; WO 02071874 A2 CAPLUS
(2) Anon; DE 10340740 A1 CAPLUS
(3) Anon; EP 1275399 A2 CAPLUS
(4) Anon; US 20060014773 A1 CAPLUS
(5) Anon: US 20060128643 A1 CAPLUS
(6) Anon; US 20060257502 A1 CAPLUS
(7) Kidd, P; Altern Med Rev 1999, V4(3), PS144
(8) McDaniel; Psychol Sci Publ Interes 2002, V3, PS12
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AN 2009:20231 CAPLUS
DN
    150:121675
    Entered STN: 08 Jan 2009
   Pyrimidine-4-carboxamide compounds useful as Raf kinase inhibitors and
     their preparation and use in the treatment of Raf-mediated diseases
     Chen, Weirong; Cossrow, Jennier; Franklin, Liovd; Guan, Bing; Jones, John
     Howard; Kumaravel, Gnanasambandam; Lane, Benjamin; Littke, Adam;
     Lugovskoy, Alexey; Peng, Hairuo; Powell, Noel; Raimundo, Brian; Tanaka,
     Hiroko; Vessels, Jeffrey; Wynn, Thomas; Xin, Zhili
     Sunesis Pharmaceuticals, Inc., USA
    PCT Int. Appl., 271pp.
     CODEN: PIXXD2
     Patent
     English
     28-16 (Heterocyclic Compounds (More Than One Hetero Atom))
     Section cross-reference(s): 1, 63
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     PATENT NO.
                         KIND
                                DATE
                                         APPLICATION NO. DATE
     WO 2009006389 A2 20090108 WO 2008-US68762 20080630
         W: AE, AG, AL, AM, AO, AT, AU, AZ, BA, BB, BG, BH, BR, BW, BY, BZ,
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             PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM,
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             TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW,
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     US 20090036419
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PRAI US 2007-947291P
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                                20070629
CLASS
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                        C07D0403-12 [I,A]; C07D0403-00 [I,C*]; C07D0401-12
                        [I,A]; C07D0401-00 [I,C*]; C07D0473-00 [I,A];
                        A61K0031-506 [I,A]; A61P0035-00 [I,A]
US 20090036419 IPCI
                       A61K0031-397 [I.A]; C07D0239-24 [I.A]; C07D0239-00
                        [I,C*]; A61K0031-505 [I,A]; C07D0295-00 [I,A];
                       C07D0473-00 [I,A]; C12N0009-99 [I,A]; A61P0009-00
                        [I,A]; A61P0037-02 [I,A]; A61P0037-00 [I,C*];
                        A61P0031-12 [I,A]; A61P0031-00 [I,C*]; A61P0019-08
                        [I,A]; A61P0019-00 [I,C*]; A61P0029-00 [I,A];
                        A61P0025-00 [I.A]; A61P0035-00 [I.A]; A61K0031-52
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                       A61K0031-5375 [I,C*]; A61K0031-496 [I,A]; A61K0031-502
                        [I,A]
                        514/210.200; 544/333.000; 514/256.000; 544/122.000;
                 NCL
                        514/235.800; 514/252.140; 514/249.000; 544/264.000;
                        514/263.210; 435/184.000
OS
    MARPAT 150:121675
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AB The invention provides compds. of formula I which are useful as inhibitors of Raf protein kinase. The invention also provides compns. thereof, and methods of treating Raf-mediated diseases. Compds. of formula I wherein Cyl is (un)substituted Ph, (un)substituted 5- to 6-membered (un)saturated heterocyclic ring; Cy2 is (un)substituted 5- to 14-membered (un)saturated or aromatic (mono/bi/tri)cyclic ring containing 0 - 4 heterocatoms; L1 is a bond and (un)substituted (un)branched Cl-6 alkylene chain; L2 is a bond and (un)substituted (un)branched Cl-6 (hetero)alkylene; R1 is H and (un)substituted Cl-6 aliphatic; Rx and Rm are independently halo, CN, OH and derivs. SH and derivs. NR2 and derivs., etc.; and pharmaceutically acceptable salts thereof, are claimed. Example compound II was prepared by a general procedure (procedure given). All the invention compds. were evaluated for their Raf-Kinase inhibitory activity (some data given).

ST pyrimidinecarboxamide prepn Raf kinase inhibitor treatment disease
IT Transplant and Transplantation

T Transplant and Transplantation (- associated diseases, treatment of; preparation of pyrimidinecarboxamide compds. as Raf kinase inhibitors useful in treatment of Raf-mediated diseases)

IT Disease, animal

(Raf-mediated, treatment of; preparation of pyrimidinecarboxamide compds. as Raf kinase inhibitors useful in treatment of Raf-mediated diseases)

IT Bone, disease

(agents for treatment of destructive, codrugs; preparation of pyrimidinecarboxamide compds. as Raf kinase inhibitors useful in treatment of Raf-mediated diseases)

IT Blood, disease

Liver, disease

(agents for treatment of, codrugs; preparation of pyrimidinecarboxamide compds. as Raf kinase inhibitors useful in treatment of Raf-mediated diseases)

T Carcinoma

Cervix, neoplasm

(cervical carcinoma, treatment of; preparation of pyrimidinecarboxamide compds. as Raf kinase inhibitors useful in treatment of Raf-mediated diseases)

IT Anti-inflammatory agents

Antidiabetic agents

Antiviral agents

Cardiovascular agents Cytotoxic agents

Immunostimulants

(codrugs; preparation of pyrimidinecarboxamide compds. as Raf kinase inhibitors useful in treatment of Raf-mediated diseases)

IT Neurotrophic factors

RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL

(Biological study); USES (Uses)

(codrugs; preparation of pyrimidinecarboxamide compds. as Raf kinase inhibitors useful in treatment of Raf-mediated diseases)

IT Intestine, neoplasm

(colon, treatment of; preparation of pyrimidinecarboxamide compds. as Raf kinase inhibitors useful in treatment of Raf-mediated diseases)

IT Nervous system, disease

(degeneration, treatment of; preparation of pyrimidinecarboxamide compds. as Raf kinase inhibitors useful in treatment of Raf-mediated diseases)

T Nerve, neoplasm

(neuroblastoma, treatment of; preparation of pyrimidinecarboxamide compds. as Raf kinase inhibitors useful in treatment of Raf-mediated diseases)

IT Thyroid gland, neoplasm

(papillary, treatment of; preparation of pyrimidinecarboxamide compds. as Raf kinase inhibitors useful in treatment of Raf-mediated diseases)

IT Antitumor agents

Combination chemotherapy

Immunomodulators

Mammalia

Mannalla Mannalla

Nervous system agents

Neuroprotective agents Pharmaceutical carriers

(preparation of pyrimidinecarboxamide compds. as Raf kinase inhibitors useful in treatment of Raf-mediated diseases)

IT Disease, animal

(proliferative, treatment of; preparation of pyrimidinecarboxamide compds. as Raf kinase inhibitors useful in treatment of Raf-mediated diseases)

IT Autoimmune disease

Bladder, neoplasm

Blood, disease Bone, disease

Bone, neoplasm

Brain, neoplasm

Cardiovascular system, disease

Cervix, neoplasm

Diabetes mellitus

Heart, disease

Immune disease

Immunodeficiency

Inflammation

Kidney, neoplasm

Larynx, neoplasm

Leukemia

Liver, disease

Lung, neoplasm

Lymphatic system, neoplasm

Lymphoma

Mammary gland, neoplasm

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Melanoma
Neuroglia, neoplasm
Ovary, neoplasm
Pancreas, neoplasm
Prostate gland, neoplasm
Stomach, neoplasm
Urogenital system, neoplasm
Viral infection
   (treatment of; preparation of pyrimidinecarboxamide compds. as Raf kinase
  inhibitors useful in treatment of Raf-mediated diseases)
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preparation); THU (Therapeutic use); BIOL (Biological study); PREP
(Preparation); RACT (Reactant or reagent); USES (Uses)
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  compds. as Raf kinase inhibitors useful in treatment of Raf-mediated
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RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic
preparation); THU (Therapeutic use); BIOL (Biological study); PREP
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RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
   (drug candidate; preparation of pyrimidinecarboxamide compds. as Raf kinase
  inhibitors useful in treatment of Raf-mediated diseases)
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RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
(Uses)
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inhibitors useful in treatment of Raf-mediated diseases) 139691-76-2, Raf kinase RL: ADV (Adverse effect, including toxicity); BSU (Biological study,

(drug candidate; preparation of pyrimidinecarboxamide compds. as Raf kinase

RL: ADV (Adverse effect, including toxicity); BSU (Biological study unclassified); BIOL (Biological study) (inhibitors; preparation of pyrimidinecarboxamide compds. as Raf kinase inhibitors useful in treatment of Raf-mediated diseases)

11 1095823-56-5P 1095823-69-0P 1095824-42-2P

RL: PEP (Physical, engineering or chemical process); RCT (Reactant); SPN

(Synthetic preparation); PREP (Preparation); PROC (Process); RACT (Reactant or reagent)

inhibitors useful in treatment of Raf-mediated diseases)
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1095824-43-3P

RL: PUR (Purification or recovery); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(intermediate; preparation of pyrimidinecarboxamide compds. as Raf kinase inhibitors useful in treatment of Raf-mediated diseases)

(intermediate; preparation of pyrimidinecarboxamide compds. as Raf kinase

368-71-8P, 1,2-Diamino-4-trifluoromethylbenzene 459-73-4P, Ethyl glycinate 949-90-6P 5305-40-8P 14160-93-1P 15030-72-5P 17321-94-7P 18202-78-3P 22808-29-3P 33142-21-1P. 2-Chloro-3-oxopropanoic acid ethyl ester 42351-88-2P 49548-40-5P 58910-26-2P 59950-56-0P 64224-60-8P 70227-49-5P 70227-50-8P 70227-51-9P 71090-35-2P, 1,1-Diamino-2-nitroethene 74667-98-4P 102999-49-5P 81587-18-0P 82353-56-8P 95080-93-6P 98024-63-6P 106615-61-6P, 4,6-Dihydroxy-5-fluoropyrimidine 118080-82-3P 141041-83-0P 213265-83-9P, 4,6-Dichloro-5-fluoropyrimidine 223788-14-5P 451491-51-3P 478259-73-3P 851984-15-1P, 4-Amino-6-chloro-5-fluoropyrimidine 863581-67-3P 872088-03-4P 893444-25-2P 893842-76-7P 914916-98-6P 939986-65-9P 1018304-56-7P 1095823-35-0P 1095823-37-2P 1095823-43-0P 1095823-45-2P 1095823-39-4P 1095823-41-8P 1095823-47-4P 1095823-50-9P 1095823-52-1P 1095823-54-3P 1095823-58-7P 1095823-60-1P 1095823-67-8P 1095823-75-8P 1095823-77-0P 1095823-79-2P 1095823-83-8P 1095823-85-0P 1095823-87-2P 1095823-91-8P 1095823-93-0P 1095823-95-2P 1095823-97-4P 1095823-99-6P 1095824-01-3P 1095824-03-5P 1095824-05-7P 1095824-08-0P 1095824-10-4P 1095824-12-6P 1095824-14-8P 1095824-16-0P 1095824-21-7P 1095824-22-8P 1095824-24-0P 1095824-25-1P 1095824-28-4P 1095824-29-5P 1095824-32-0P 1095824-33-1P 1095824-34-2P 1095824-35-3P 1095824-36-4P 1095824-37-5P 1095824-38-6P 1095824-39-7P 1095824-40-0P 1095824-41-1P 1095824-45-5P 1095824-46-6P 1095824-47-7P 1095824-48-8P 1095824-50-2P 1095824-51-3P 1095824-52-4P 1095824-53-5P 1095824-54-6P 1095824-55-7P 1095824-56-8P 1095824-57-9P 1095824-58-0P 1095824-59-1P 1095824-67-1P 1095824-68-2P 1095825-41-4P 1095825-71-0P 1097250-57-1P 1097250-58-2P 1097250-61-7P 1097250-62-8P 1097250-65-1P 1097250-66-2P 1097250-69-5P 1097250-71-9P 1097250-73-1P 1097250-75-3P 1097250-77-5P 1097250-79-7P 1097250-82-2P 1097250-84-4P 1097250-86-6P 1097250-90-2P 1097250-92-4P 1097250-94-6P 1097250-95-7P 1097250-98-0P 1097251-04-1P 1097251-06-3P 1097251-07-4P 1097251-09-6P 1097251-12-1P 1097251-14-3P 1097251-16-5P 1097251-17-6P 1097251-21-2P 1097251-23-4P 1097251-26-7P 1097251-28-9P 1097251-29-0P 1097251-31-4P 1097251-33-6P 1097251-36-9P 1097251-38-1P 1097251-43-8P 1097251-45-0P 1097251-48-3P 1097251-50-7P 1097252-41-9P 1097252-46-4P 1097252-49-7P 1097251-50-7P 1097251-52-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(intermediate; preparation of pyrimidinecarboxamide compds. as Raf kinase inhibitors useful in treatment of Raf-mediated diseases) 144697-16-5, B-Raf kinase

RL: ADV (Adverse effect, including toxicity); BSU (Biological study, unclassified); BIOL (Biological study)

(preparation of pyrimidinecarboxamide compds. as Raf kinase inhibitors

useful in treatment of Raf-mediated diseases)

IT 142805-58-1, MEK1 KINASE 146702-84-3 150316-14-6, MEK2 KINASE

RL: BSU (Biological study, unclassified); BIOL (Biological study)

(preparation of pyrimidinecarboxamide compds. as Raf kinase inhibitors useful in treatment of Raf-mediated diseases)

IT 1095824-44-4P

RL: PUR (Purification or recovery); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of pyrimidinecarboxamide compds. as Raf kinase inhibitors useful in treatment of Raf-mediated diseases)

IT 1097257-17-4P

ΤТ

RL: BYP (Byproduct); PRPH (Prophetic); PREP (Preparation)

(prophetic byproduct; preparation of pyrimidinecarboxamide compds. as Raf kinase inhibitors useful in treatment of Raf-mediated diseases)

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                              1096362-00-3P
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1096362-02-5P
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1096362-06-9P
RL: PAC (Pharmacological activity); PRPH (Prophetic); SPN (Synthetic
preparation); THU (Therapeutic use); BIOL (Biological study); PREP
(Preparation); USES (Uses)
   (prophetic drug candidate; preparation of pyrimidinecarboxamide compds. as
  Raf kinase inhibitors useful in treatment of Raf-mediated diseases)
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TТ

1096363-98-2P

1096363-99-3P

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RL: PAC (Pharmacological activity); PRPH (Prophetic); SPN (Synthetic
preparation); THU (Therapeutic use); BIOL (Biological study); PREP
(Preparation); USES (Uses)
   (prophetic drug candidate; preparation of pyrimidinecarboxamide compds. as
   Raf kinase inhibitors useful in treatment of Raf-mediated diseases)
1095825-44-7P
RL: PRPH (Prophetic); PUR (Purification or recovery); RCT (Reactant); SPN
(Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
   (prophetic drug candidate; preparation of pyrimidinecarboxamide compds. as
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6299-87-2P, 6-Hydroxypyrimidine-4-carboxylic acid 28668-32-8P
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873009-27-9P
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              933728-94-0P
                            933731-47-6P 933753-44-7P
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RL: PRPH (Prophetic); RCT (Reactant); SPN (Synthetic preparation); PREP
(Preparation); RACT (Reactant or reagent)
   (prophetic intermediate; preparation of pyrimidinecarboxamide compds. as Raf
   kinase inhibitors useful in treatment of Raf-mediated diseases)
61-82-5, 1H-1,2,4-Triazol-5-amine 62-53-3, Aniline, reactions 62-57-7,
2-Amino-2-methylpropanoic acid 71-36-3, 1-Butanol, reactions 75-31-0,
Isopropylamine, reactions 75-97-8, tert-Butyl methyl ketone 75-98-9,
Pivalic acid 78-95-5, Chloroacetone 96-50-4, 2-Aminothiazole
96-98-0, 4-Methyl-3-nitrobenzoic acid 98-16-8, 3-Trifluoromethylaniline
100-46-9, Benzylamine, reactions 103-76-4, 1-(2-Hydroxyethyl)piperazine
104-78-9, N,N-Diethylpropane-1,3-diamine 105-36-2, Ethyl 2-bromoacetate
105-39-5, Ethyl chloroacetate 106-47-8, 4-Chloroaniline, reactions
107-10-8, n-Propylamine, reactions 107-19-7, Propargyl alcohol
108-00-9, N, N-Dimethylethylenediamine 108-01-0, 2-
Dimethylaminoethanol 108-42-9, 3-Chloroaniline 109-00-2, 3-Pyridinol 109-01-3, 1-Methylpiperazine 109-12-6, 2-Pyrimidinamine
109-55-7, N,N-Dimethyl-1,3-propanediamine 109-85-3, 2-Methoxyethylamine
109-94-4, Ethyl formate 109-97-7, Pyrrole 110-89-4, Piperidine, reactions 110-91-8, Morpholine, reactions
4-Methyl-3-nitroaniline 121-01-7, 4-Nitro-2-trifluoromethylaniline
123-00-2, N-(3-Aminopropyl)morpholine 123-75-1, Pyrrolidine, reactions
141-30-0, 3,6-Dichloropyridazine 141-78-6, Ethyl acetate, reactions
156-87-6, 3-Aminopropanol 288-13-1, Pyrazole 288-32-4, Imidazole,
reactions 320-51-4, 4-Chloro-3-trifluoromethylaniline 328-80-3
349-81-5 400-98-6, 2-Nitro-4-trifluoromethylaniline 426-59-5,
3-Trifluoromethylsulfonylaniline 445-13-6,
3-Chloro-4-trifluoromethylaniline 455-14-1, 4-Trifluoromethylaniline
462-08-8, 3-Pyridinamine 488-11-9, Mucobromic acid 504-24-5,
4-Aminopyridine 504-29-0, 2-Aminopyridine 591-54-8, 4-Pyrimidinamine
613-89-8, 2-Amino-1-phenylethanone 616-30-8, 3-Aminopropane-1,2-diol
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2,2-Dimethylpropanenitrile
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                                      685-88-1, Diethyl fluoromalonate
693-98-1, 2-Methylimidazole 762-21-0, Diethyl acetylenedicarboxylate
769-92-6, 4-tert-Butylaniline 822-36-6, 4-Methylimidazole
3-Butvn-1-ol 1001-53-2, N-Acetvlethylenediamine 1186-70-5,
Methoxy-bis(dimethylamino)methane 1193-24-4, 4,6-Dihydroxypyrimidine
1453-58-3, 3-Methylpyrazole 1567-75-5, 1-Acetyl-1-methylcyclopropane
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1736-72-7 1737-36-6, 4-Chloro-3-trifluoromethylbenzoic acid 1750-42-1,
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3-Dimethylaminopropanol 3435-27-6 3731-52-0, 3-Pyridinemethanamine
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4572-03-6, 1-(3-Aminopropyl)-4-methylpiperazine 4726-85-6,
                                                           5049-61-6,
3-Aminopropanamide 5036-48-6, N-(3-Aminopropyl)imidazole
2-Pyrazinamine 5098-11-3 5292-43-3, tert-Butyl bromoacetate
5308-25-8, N-Ethylpiperazine 5369-19-7, 3-tert-Butylaniline 5382-16-1,
4-Piperidinol 5390-04-5, 4-Pentyn-1-ol 5623-95-0,
1-Piperazinecarboxamide 5625-67-2, Piperazinone 5654-83-1 6271-78-9,
6-Chloropyridine-3-carboxamide 6291-85-6, 3-Ethoxypropylamine
6457-49-4, 4-Piperidinemethanol 6627-22-1 6628-77-9,
6-Methoxypyridin-3-amine 7149-42-0, 4-Aminomethyl-1-methylpiperidine
7663-77-6, N-(3-Aminopropyl)pyrrolidin-2-one 7720-39-0,
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1H-Imidazol-2-amine 13035-19-3, 4-Piperidinamine 13139-17-8,
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13484-38-3
           13623-94-4, 1,1-Bis(methylthio)-2-nitroethene 16490-02-1,
4.6-Pvrimidinedicarboxvlic acid 20265-38-7, 2-Methoxypvridin-3-amine
20566-90-9 21717-96-4, 2-Amino-5-fluoropyridine 22059-21-8,
1-Aminocyclopropanecarboxylic acid 22195-47-7 22356-89-4
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Aminoacetaldehyde dimethyl acetal 23159-07-1,
N-(3-Aminopropyl)pyrrolidine 25057-77-6, 1,2-Dimethylpiperazine
27578-60-5, 1-Piperidineethanamine 31462-59-6, 4-Pvrimidinecarboxvlic
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40499-83-0, 3-Pyrrolidinol 41661-47-6, 4-Piperidinone
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4-Amino-1-methylpiperidine 49750-74-5,
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2-(2-Aminoethyl)-1-methylpyrrolidine 51940-63-7 55338-73-3,
3-Amino-6-cyanopyridine 55676-22-7, 1-(6-Chloropyridin-3-yl)ethanone
55809-36-4, 3-Amino-5-tert-butylisoxazole 57260-71-6, N-Boc-piperazine
58757-38-3, 6-Chloropyridine-3-carbonyl chloride 65934-74-9,
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4-Mmino-l-(tert-Dutoxycarbonylamino)actaldehyde 99724-19-3,
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173340-26-6 181219-01-2, 4-(4,4,5,5-Tetramethyl-[1,3,2]dioxaborolan-2-
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186550-13-0, tert-Butvl 3-aminopyrrolidine-1-carboxylate 214701-31-2
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RL: RCT (Reactant); RACT (Reactant or reagent)
   (starting material; preparation of pyrimidinecarboxamide compds. as Raf
  kinase inhibitors useful in treatment of Raf-mediated diseases)
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ANSWER 4 OF 55 CAPLUS COPYRIGHT 2009 ACS on STN

AN 2008:1530405 CAPLUS

DN 150:77500

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ED Entered STN: 24 Dec 2008

- TI 2-Aminothiophene-3-carboxamide derivatives as inhibitors of janus kinases and their preparation and use in the treatment of myeloproliferative disorders and cancers
- IN Altman, Michael; Christopher, Matthew; Grimm, Jonathan B.; Haidle, Andrew; Konrad, Kaleen; Lim, Jongwon; Maccoss, Rachel N.; Machacek, Michelle; Osimboni, Ekundayo; Otte, Ryan D.; Siu, Tony; Spencer, Kerrie; Taoka, Brandon; Tempest, Paul; Wilson, Kevin; Woo, Hyun Chong; Young, Jonathan; Zabierek, Anna
- PA Merck & Co., Inc., USA
- SO PCT Int. Appl., 511pp.
- CODEN: PIXXD2
- DT Patent
- LA English
- CC 27-8 (Heterocyclic Compounds (One Hetero Atom)) Section cross-reference(s): 1, 63

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WO	WO 2008156726			IPC				3-06 [I,A]; A01N0043-02 [I,C*]; A61K0031-38 A61K0031-535 [I,A]									38	

MARPAT 150:77500 os

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- The invention provides compds. of formula I that inhibit the four known mammalian JAK kinases (JAK1, JAK2, JAK3 and TYK2) and PDK1. The invention also provides for compns. comprising such inhibitory compds. and methods of inhibiting the activity of JAK1, JAK2, JAK3 TYK2 and PDK1 by administering the compound to a patient in need of treatment for myeloproliferative disorders or cancer. Compds. of formula I wherein W is N and CR4; Y is N and CR3; Z is N and CR2; R1 and R2 are independently H, halo, CN, (un) substituted C1-3 alkyl; R3 is H, halo, CN, Oxo, C1-6 alkyl, C2-6 alkynyl, etc.; R5 is H, halo, CN, oxo, NH2 and derivs., etc.; R5 is (un) substituted (hetero) aryl; and pharmaceutically acceptable salts and stereoisomers thereof, are claimed. Example compound II was prepared by arylation of 2-amino-5-(2,4-difluorophenyl)thiophene-3-carboxamide with (6-bromopyridin-2-yl) methanol. All the invention compds. were evaluated for their janus kinase inhibitory activity (some data given).
- aminothiophenecarboxamide prepn janus kinase inhibitor treatment myeloproliferative disorder cancer
- Antitumor agents

Mammalia

Pharmaceutical carriers

(preparation of aminothiophenecarboxamide derivs. as janus kinase inhibitors

useful in the treatment of myeloproliferative disorders and cancer)

T Myeloproliferative disorders

Neoplasm

(treatment of; preparation of aminothiophenecarboxamide derivs. as janus kinase inhibitors useful in the treatment of myeloproliferative disorders and cancer)

IT 1093872-09-3P 1093872-14-0P

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP

(Preparation); RACT (Reactant or reagent); USES (Uses) (drug candidate and intermediate; preparation of aminothiophenecarboxamide derivs. as janus kinase inhibitors useful in the treatment of

myeloproliferative disorders and cancer)

1093873-15-4P 1093873-18-7P 1093876-04-0P 1093876-18-6P RL: PAC (Pharmacological activity); PEP (Physical, engineering or chemical process); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); PROC (Process); USES (Uses)

(drug candidate; preparation of aminothiophenecarboxamide derivs. as janus kinase inhibitors useful in the treatment of myeloproliferative disorders and cancer)

IT 1093873-17-6P 1093873-19-8P 1093873-20-1P 1093877-12-3P 1093877-90-7P 1093877-91-8P 1093877-92-9P 1093877-93-0P 1093877-95-2P

RL: PAC (Pharmacological activity); PUR (Purification or recovery); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(drug candidate; preparation of aminothiophenecarboxamide derivs. as janus kinase inhibitors useful in the treatment of myeloproliferative disorders and cancer)

	disorders an	nd cancer)		
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RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
(Uses)
  (drug candidate; preparation of aminothiophenecarboxamide derivs. as janus
  kinase inhibitors useful in the treatment of myeloproliferative
  disorders and cancer)
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                              1093876-38-0P
                                              1093876-39-1P
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                              1093876-42-6P
1093876-44-8P 1093876-45-9P
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RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(drug candidate; preparation of aminothiophenecarboxamide derivs. as janus kinase inhibitors useful in the treatment of myeloproliferative

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disorders and cancer)
1093876-46-0P 1093876-47-1P
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1093876-50-6P 1093876-51-7P
                            1093876-52-8P 1093876-53-9P
1093876-54-0P 1093876-55-1P 1093876-56-2P 1093876-57-3P
1093876-58-4P 1093876-59-5P 1093876-60-8P 1093876-61-9P
1093876-62-0P 1093876-63-1P 1093876-64-2P 1093876-65-3P
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1093876-70-0P 1093876-71-1P 1093876-72-2P 1093876-73-3P
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             1093877-00-9P
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1093877-32-7P
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                              1093877-34-9P
                                             1093877-35-0P
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                                            1093877-43-0P
1093877-44-1P 1093877-45-2P 1093877-46-3P 1093877-47-4P
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1093877-52-1P 1093877-53-2P
                            1093877-54-3P 1093877-55-4P
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                              1093877-70-3P 1093877-71-4P
1093877-72-5P 1093877-73-6P
                              1093877-74-7P 1093877-75-8P
1093877-76-9P 1093877-77-0P
                             1093877-78-1P 1093877-79-2P
1093877-80-5P 1093877-81-6P
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1093877-84-9P 1093877-85-0P
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RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
(Uses)
  (drug candidate; preparation of aminothiophenecarboxamide derivs. as janus
  kinase inhibitors useful in the treatment of myeloproliferative
  disorders and cancer)
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27217-81-8P 33674-94-1P 33852-01-6P
                                      41036-01-5P
                                                   54864-83-4P
61019-14-5P 61019-15-6P
                         61019-17-8P
                                                    64128-11-6P
                                      61396-73-4P
65515-32-4P 66909-36-2P, 6-Chloro-2-methylnicotinonitrile 70291-28-0P
74134-42-2P 74649-06-2P 76013-48-4P 79039-86-4P 83004-10-8P 83774-09-8P 98626-92-7P 102877-36-1P 111991-19-6P 112575-11-8P
             118775-68-1P
139163-56-7P
142978-11-8P
176661-75-9P
2630
118078-88-9P 118775-68-1P 118863-62-0P 129601-00-9P
                                                        131653-51-5P
                            142978-11-8P
                                                         153976-27-3P
137129-98-7P
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168038-14-0P
             176249-43-7P
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1H-Pvrazole-4-ethanol 258506-70-6P 263012-63-1P 286961-15-7P
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4-Bromo-2,6-difluorobenzaldehyde 570398-18-4P 588689-47-8P
638218-78-7P 675109-37-2P 736991-31-4P 743438-38-2P,
2-Azaspiro[3.3]heptane-2-ethanol 848953-11-7P 851759-19-8P
859849-55-1P 871239-58-6P 872700-68-0P 898044-48-9P 914360-19-3P
936940-67-9P 945892-89-7P 945947-99-9P,
3-0xa-1,8-diazaspiro[4,5]decan-2-one 955370-07-7P 959237-45-7P
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                              1093878-58-0P
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                              1093878-66-0P 1093878-67-1P
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                              1093878-70-6P 1093878-71-7P
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1093878-96-6P 1093878-97-7P 1093878-98-8P 1093878-99-9P
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1093879-04-9P
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                                               1093879-07-2P
1093879-08-3P
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                                               1093879-11-8P
1093879-12-9P
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                               1093879-14-1P
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1093879-20-9P
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                               1093879-26-5P
                                               1093879-27-6P
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                                               1093879-39-0P
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                               1093879-42-5P
                                               1093879-43-6P
1093879-44-7P
              1093879-45-8P
                               1093879-46-9P
                                               1093879-47-0P
1093879-48-1P
              1093879-49-2P
                              1093879-50-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
   (intermediate; preparation of aminothiophenecarboxamide derivs. as janus
  kinase inhibitors useful in the treatment of myeloproliferative
  disorders and cancer)
1093879-51-6P
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                               1093879-53-8P
                                               1093879-54-9P
1093879-55-0P
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                               1093879-57-2P
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1093879-59-4P
1093879-63-0P
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                               1093879-65-2P
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                                               1093879-70-9P
1093879-67-4P
               1093879-68-5P
                               1093879-69-6P
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               1093879-72-1P
                               1093879-73-2P
                                               1093879-74-3P
1093879-75-4P
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                               1093879-77-6P
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                                               1093879-86-7P
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                               1093879-89-0P
                                               1093879-90-3P
1093879-91-4P
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                               1093879-93-6P
                                              1093879-94-7P
1093879-95-8P
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                                              1093880-03-5P
1093879-99-2P
               1093880-01-3P
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                               1093880-06-8P
                                              1093880-07-9P
1093880-08-0P
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1093881-23-2P 1093881-24-3P

1093881-27-6P 1093881-28-7P

1093881-21-0P 1093881-22-1P

1093881-26-5P

1093881-25-4P

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1093881-29-8P 1093881-30-1P 1093881-31-2P 1093881-32-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
   (intermediate; preparation of aminothiophenecarboxamide derivs, as janus
  kinase inhibitors useful in the treatment of myeloproliferative
  disorders and cancer)
152478-56-3, Janus kinase 1
                            152478-57-4, Janus kinase 2 153190-61-5,
TYK2 kinase 157482-36-5, Janus kinase 3 161384-16-3, Janus kinase
191808-15-8, Phosphoinositide dependent protein kinase 1
RL: BSU (Biological study, unclassified); BIOL (Biological study)
   (preparation of aminothiophenecarboxamide derivs. as janus kinase inhibitors
  useful in the treatment of myeloproliferative disorders and cancer)
1093876-99-3P
RL: PAC (Pharmacological activity); PEP (Physical, engineering or chemical
process); SPN (Synthetic preparation); THU (Therapeutic use); BIOL
(Biological study); PREP (Preparation); PROC (Process); USES (Uses)
   (preparation of aminothiophenecarboxamide derivs. as janus kinase inhibitors
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useful in the treatment of myeloproliferative disorders and cancer)
11 1093873-16-59
RI: PAC (Pharmacological activity); PUR (Purification or recovery); SPN
(Synthetic preparation); THU (Therapeutic use); BIOL (Biological study);

(Synthetic preparation); THU (Therapeutic use); BIOL (Biological study);
PREP (Preparation); USES (Uses)
(oreoaration of aminothiophenecarboxamide derivs. as janus kinase inhibitors

useful in the treatment of myeloproliferative disorders and cancer)

[T 1093880-00-2P

RL: SPN (Synthetic preparation); PREP (Preparation)

(product; preparation of aminothiophenecarboxamide derivs. as janus kinase inhibitors useful in the treatment of myeloproliferative disorders and cancer)

IT 75867-44-6P

ΙT

RL: BYP (Byproduct); PRPH (Prophetic); PREP (Preparation) (prophetic byproduct; preparation of aminothiophenecarboxamide derivs. as janus kinase inhibitors useful in the treatment of myeloproliferative disorders and cancer)

disorders and cancer)

11 27-06-0P 5382-89-8P 55368-83-7P 86941-36-8P 85579-92-0P
8985-31-2P 90792-83-9P 138647-49-1P 168038-13-9P 169297-84-1P
177940-20-4P 186294-80-4P 186294-83-7P 445468-65-5P 518047-39-7P
845488-74-4P, 3-Morpholinecarboxamide 1004517-04-7P 1083169-01-0P
1093881-56-1P 1093881-57-2P 1093881-58-3P 1093881-59-4P
1093881-60-7P 1093881-61-8P 1093881-62-9P 1093881-50-0P
1093881-64-1P 1093881-61-8P 1093881-66-3P
RL: PRPH (Prophetic); RCT (Reactant); SPN (Synthetic preparation); PREF
(Preparation); RACT (Reactant or reagent)
(prophetic intermediate; preparation of aminothiophenecarboxamide derivs. as janus kinase inhibitors useful in the treatment of myeloproliferative disorders and cancer)

67-64-1, Acetone, reactions 75-31-0, Isopropylamine, reactions 75-33-2, Isopropylthiol 75-65-0, 2-Methylpropan-2-ol, reactions 75-66-1, tert-Butylthiol 77-77-0, Divinyl sulfone 78-82-0, 2-Methylpropanenitrile 78-84-2, Isobutyraldehyde 78-96-6. 2-Hydroxypropylamine 96-32-2, Methyl bromoacetate 96-35-5, Methyl hydroxyacetate 96-50-4, 2-Aminothiazole 98-59-9, Tosyl chloride 100-72-1, 2-Tetrahydropyranmethanol 104-63-2, 2-Benzylaminoethanol 105-36-2, Ethyl bromoacetate 106-37-6, 1,4-Dibromobenzene 106-40-1, 4-Bromoaniline 106-95-6, Allyl bromide, reactions 1-Propanethiol 107-91-5, Cyanoacetamide 108-00-9, 107-03-9. N,N-Dimethylethylenediamine 108-01-0, 2-Dimethylaminoethanol 109-01-3, 1-Methylpiperazine 109-11-5, 3-Morpholinone 109-59-1, 2-Isopropoxyethanol 109-78-4, 3-Hydroxypropanenitrile 109-83-1, N-Methyl-2-hydroxyethylamine 109-85-3, 2-Methoxyethylamine 109-94-4,

Ethyl formate 110-89-4, Piperidine, reactions 110-91-8, Morpholine, reactions 111-42-2, Bis(2-hydroxyethyl)amine, reactions

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115-19-5, 2-Methylbut-3-yn-2-ol 120-93-4, 2-Imidazolidinone 122-51-0,
Ethyl orthoformate 123-11-5, 4-Methoxybenzaldehyde, reactions
123-75-1, Pyrrolidine, reactions 141-30-0, 3,6-Dichloropyridazine 141-91-3, 2,6-Dimethylmorpholine 288-13-1, Pyrazole 288-32-4,
Imidazole, reactions 288-36-8, 1H-1,2,3-Triazole 352-13-6,
4-Fluorophenylmagnesium bromide 431-38-9 459-56-3, 4-Fluorobenzyl
alcohol 459-73-4 461-96-1, 1-Bromo-3,5-difluorobenzene 497-25-6,
2-Oxazolidinone 501-53-1, Benzyloxycarbonyl chloride 503-29-7,
Azetidine 504-02-9, 1,3-Cvclohexanedione 513-44-0, Isobutvlthiol
558-30-5, 1,2-Epoxy-2-methylpropane 586-95-8, 4-Pyridinemethanol
609-36-9, Proline 616-45-5, 2-Pyrrolidinone 619-44-3, Methyl
4-iodobenzoate 623-00-7, 4-Bromobenzonitrile 623-33-6, Glycine ethyl
ester hydrochloride 623-51-8, Ethyl mercaptoacetate 624-28-2,
2,5-Dibromopyridine 624-78-2, N-Methylethylamine 626-05-1,
2,6-Dibromopyridine 637-81-0, Ethyl azidoacetate 922-67-8, Methyl
propiolate 927-74-2, 3-Butyn-1-ol 930-46-1 1066-54-2,
Trimethylsilylacetylene 1072-86-2 1074-82-4, Potassium phthalimide
1192-21-8, 1-Methyl-1H-pyrazol-5-ylamine 1192-81-0,
                                          1489-69-6,
5-Chloromethyl-3-methyl-1,2,4-oxadiazole
Cyclopropanecarboxaldehyde 1692-25-7, Pyridin-3-ylboronic acid
1745-18-2, 1-Ally1-4-chlorobenzene 1792-81-0 1857-19-8 1857-20-1 1904-31-0, 3-Amino-1-methylpyrazole 1993-03-9, 2-Fluorophenylboronic
     2240-88-2 2483-65-0, 3-Aminopyrrolidin-2-one 2516-33-8,
Cyclopropylmethanol 2516-47-4, Cyclopropylmethylamine 2749-11-3,
($)-2-Aminopropan-1-ol 2799-17-9 2854-16-2 2916-68-9, 2-Trimethylsilylethanol 3218-02-8, Aminomethylcyclohexane
                                                               3433-37-2.
2-(Hydroxymethyl)piperidine 3699-54-5 3779-29-1, Diethyl
cyclobutane-1,1-dicarboxylate 3859-41-4, 1,3-Cyclopentanedione
3914-42-9, 2-Chloromethyl-5-methyl-1,3,4-oxadiazole 3921-01-5,
2,4-Dibromopyrimidine 3934-20-1, 2,4-Dichloropyrimidine 4254-15-3,
reactions 4358-64-9 4415-82-1, Cyclobutanemethanol 4637-24-5
4651-82-5, 2-Amino-3-cyanothiophene 4795-29-3,
2-Aminomethyltetrahydrofuran 5057-98-7 5076-19-7,
2,2,3-Trimethyloxirane 5193-03-3, 2-Chloro-6-hydrazinopyridine
5315-25-3, 2-Bromo-6-methylpyridine 5382-16-1, 4-Piperidinol
5464-12-0, 1-(2-Hydroxyethyl)-4-methylpiperazine 5675-32-1 6317-37-9,
5-Nitrothiophene-2-carboxylic acid 6338-70-1,
3-Aminotetrahydrothiophene-1,1-dioxide 6361-23-5,
2,5-Dichlorobenzaldehyde 6457-49-4, 4-Piperidinemethanol 6482-24-2,
1-Bromo-2-methoxyethane 6704-31-0, 3-Oxetanone 6705-33-5,
Pyrazinemethanol 6952-93-8 13195-50-1, 2-Bromo-5-nitrothiophene
13889-98-0, N-Acetylpiperazine 14080-51-4,
2-Aminothiophene-3-carboxamide 14716-89-3,
5-Hydroxymethyl-3-methylisoxazole 14916-79-1, 3-Heptyn-1-ol
15205-66-0, 2-Methylsulfonylethanol 15833-61-1,
3-Tetrahydrofuranmethanol 18997-19-8, Chloromethyl pivalate
20885-12-5, 2-Chloro-6-fluoropyridine 21190-87-4,
6-Bromopyridine-2-carboxylic acid 21635-88-1, 3-Aminooxetane
21987-29-1, 4,4-Difluoropiperidine 22677-21-0 23100-12-1,
6-Chloronicotinaldehyde 23804-68-4, 4-Aminomethyl-1-benzylpiperidin-4-ol
25016-11-9, 1-Methylpyrazole-4-carboxaldehyde
                                               29683-23-6,
Tetrahydrothiopyran-4-ol 29943-42-8, Tetrahydropyran-4-one
                                                                31181-79-0
31329-64-3, 4-Amino-3,5-dimethylisoxazole 33674-96-3 34160-40-2,
6-Bromopyridine-2-carboxaldehyde 34368-52-0 35320-23-1 39093-93-1,
Thiomorpholine dioxide 40499-83-0, 3-Pyrrolidinol 42839-09-8,
2-Pyrimidinemethanol 45347-82-8, 3-Azetidinol 45513-32-4,
3-Aminomethyl-3-hydroxymethyloxetane 49669-13-8,
1-(6-Bromopyridin-2-y1)ethanone 49773-20-8, 2-Methylsulfonylethylamine
50382-32-6, 2,4-Dimethylthiazole-5-methanol 50534-49-1,
3-Dimethylaminopiperidine 50606-31-0 50675-19-9,
Tetrahydro-2H-thiopyran-4-carboxaldehyde 50910-54-8,
trans-4-Aminocyclohexanol hydrochloride 54042-97-6,
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59702-07-7, 1-Methylpiperazin-2-one 61676-62-8,
    2-Isopropoxy-4,4,5,5-tetramethyl-1,3,2-dioxaborolane 65202-50-8, Methyl
    6-chloropyridazine-3-carboxylate 65412-03-5,
    4-(2-Aminoethyl)tetrahydropyran 65515-28-8, Methyl
    2.6-dichloronicotinate 65719-09-7, Methyl 2-methylpyridine-3-carboxylate
    66389-76-2 68108-18-9 69843-13-6 73183-34-3 74572-04-6
    79286-79-6, 3-Aminopyrrolidine 81971-39-3,
    5-Bromo-1-methylpyridin-2(1H)-one 86864-60-0 87576-94-1,
    Trimethylsilvlmethyl azide 91476-80-1,
    5,6,7,8-Tetrahydroimidazo[1,2-a]pyrazine
                                             92136-39-5 102065-86-1,
    3-Aminoazetidine 103003-01-6, 2-(Hydroxymethyl)morpholine 103775-61-7
    106910-83-2, 3-(Hydroxymethyl)morpholine 107017-72-1 109074-67-1,
    2-Trifluoromethylpyrrolidine 110925-17-2, 3-Methoxyazetidine
    112575-15-2, 2-Bromo-6-methoxymethylpyridine 112960-56-2 115845-51-7
    119329-48-5 120099-60-7, (R)-3-Methoxypyrrolidine 120099-61-8
    120739-79-9 125295-22-9 130290-79-8, 4-Aminomethyltetrahydropyran
    130551-92-7, 2-0xazolemethanol 132995-76-7, 2-(2-Hydroxyethyl)morpholine
    136725-54-7, (S)-3-Fluoropyrrolidine 137641-74-8 141567-42-2 141699-55-0, 1-(tert-Butoxycarbonyl)-azetidin-3-01 144025-03-6,
    2,4-Difluorophenylboronic acid 149104-90-5, 4-Acetylphenylboronic acid
     153209-97-3, 3-Aminomethyl-3-methyloxetane 155732-68-6 158780-91-7
     164666-68-6, 6-Chloro-2-methylpyridin-3-amine 165253-31-6,
    3-Aminomethyltetrahydrofuran 165736-07-2 212650-43-6 263012-81-3
    288315-03-7, 3,3-Difluoroazetidine hydrochloride 289037-48-5,
    3-Azabicyclo[3.1.0]hexane-6-methanol 290307-40-3,
    2-(5-Bromopyridin-2-y1)propan-2-ol 316131-01-8, 3,3-Difluoropyrrolidine
    332134-60-8 363179-66-2, 3,3-Difluoropiperidine 374776-56-4
    376584-63-3 400877-05-6
                               433980-62-2, 3-Methylsulfonylpyrrolidine
    444120-91-6 477904-80-6, Cyclopropanecarboximidamide hydrochloride
    485799-04-0 552846-17-0 603143-27-7 612511-81-6 679431-52-8,
    3.3-Difluoroazetidine 761446-44-0 847818-74-0 852227-86-2
    852228-08-1 863548-52-1 884495-36-7 885273-36-9
    RL: RCT (Reactant); RACT (Reactant or reagent)
        (starting material; preparation of aminothiophenecarboxamide derivs. as
       janus kinase inhibitors useful in the treatment of myeloproliferative
       disorders and cancer)
    885280-56-8 885331-17-9, 2-Oxazolemethanamine
                                                    914947-26-5
    915920-22-8 933745-16-5 936940-63-5 944902-13-0 945459-80-3
    1073355-02-8 1093881-33-4 1093881-34-5 1093881-35-6 1093881-36-7
    1093881-37-8 1093881-38-9 1093881-39-0 1093881-40-3 1093881-41-4
    1093881-42-5 1093881-43-6 1093881-44-7 1093881-45-8 1093881-46-9
    1093881-47-0 1093881-48-1 1093881-49-2 1093881-50-5 1093881-54-9
    1093881-55-0
    RL: RCT (Reactant): RACT (Reactant or reagent)
        (starting material; preparation of aminothiophenecarboxamide derivs. as
        janus kinase inhibitors useful in the treatment of myeloproliferative
       disorders and cancer)
    1060642-93-4 1093959-48-8
    RL: PRP (Properties)
        (unclaimed sequence: 2-Aminothiophene-3-carboxamide derivs. as
        inhibitors of janus kinases and their preparation and use in the treatment
       of myeloproliferative disorders and cancers)
RE.CNT 3
             THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD
(1) Adams; US 7179836 B2 2007 CAPLUS
(2) Bloxham: US 20050154014 A1 2005 CAPLUS
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5-(Chloromethyl)-3-isopropyl-1,2,4-oxadiazole 55261-00-2 55276-43-2,

2,4,6-Trifluorobenzaldehyde 58757-38-3, 6-Chloronicotinoyl chloride

3-Methoxy-3-methylbutanol 57012-20-1 57260-73-8, N-Boc-ethylenediamine 57848-46-1, 4-Bromo-2-fluorobenzaldehyde 58551-83-0,

1-Methylsulfonylpiperazine 56414-96-1 56539-66-3,

57611-57-1

(3) Ushio; US 7112594 B2 2006 CAPLUS

- ANSWER 5 OF 55 CAPLUS COPYRIGHT 2009 ACS on STN 1.9
- AN 2008:1402558 CAPLUS
- 149 585299 DN
- Entered STN: 21 Nov 2008 ED
- TΙ A gum solution for developing and gumming a photopolymer printing plate.
- IN Gries, Willi-Kurt; Hendrikx, Peter; Van Damme, Marc
- PA Agfa Graphics NV, Belg.
- SO PCT Int. Appl., 61pp.
 - CODEN: PIXXD2
- DT Patent
- LA English
- CC 74-6 (Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes)

FAN.CNT 1																			
PATENT NO.					KIND		DATE			APPL	ICAT:		DATE						
PI	WO	2008138942			A1 200			20081120			WO 2008-EP55872					20080514			
		W:	ΑE,	AG,	AL,	AM,	AO,	AT,	AU,	ΑZ,	BA,	BB,	BG,	BH,	BR,	BW,	BY,	ΒZ,	
			CA,	CH,	CN,	CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DO,	DZ,	EC,	EE,	EG,	ES,	
			FI,	GB,	GD,	GE,	GH,	GM,	GT,	HN,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	KE,	
			KG,	KM,	KN,	KP,	KR,	KZ,	LA,	LC,	LK,	LR,	LS,	LT,	LU,	LY,	MA,	MD,	
			ME,	MG,	MK,	MN,	MW,	MX,	MY,	MZ,	NA,	NG,	NI,	NO,	NZ,	OM,	PG,	PH,	
			PL,	PT,	RO,	RS,	RU,	SC,	SD,	SE,	SG,	SK,	SL,	SM,	SV,	SY,	TJ,	TM,	
			TN,	TR,	TT,	TZ,	UA,	UG,	US,	UZ,	VC,	VN,	ZA,	ZM,	ZW				
		RW:	ΑT,	BE,	BG,	CH,	CY,	CZ,	DE,	DK,	EE,	ES,	FI,	FR,	GB,	GR,	HR,	HU,	
			ΙE,	IS,	IT,	LT,	LU,	LV,	MC,	MT,	NL,	NO,	PL,	PT,	RO,	SE,	SI,	SK,	
			TR,	BF,	ВJ,	CF,	CG,	CI,	CM,	GA,	GN,	GQ,	GW,	ML,	MR,	NE,	SN,	TD,	
			TG,	BW,	GH,	GM,	KE,	LS,	MW,	MZ,	NA,	SD,	SL,	SZ,	TZ,	UG,	ZM,	ZW,	
			AM,	AZ,	BY,	KG,	KZ,	MD,	RU,	TJ,	TM								
PRAI	EP	2007-108228			A		2007	0515											
	US	2007-938015P			P		2007	0515											

CLASS PATENT NO. CLASS PATENT FAMILY CLASSIFICATION CODES

WO 2008138942 IPCI G03F0007-32 [I.A]

A gum solution is provided which comprises a film forming hydrophilic polymer or surfactant, and a salt formed by reaction of an acid, selected from phosphoric acid and phosphorous acid, with a di- or tri-alkanolamine. The qum solution is suitable for developing and qumming a lithog, photopolymer printing plate precursor. Also provided is a method for preparing a lithog. printing plate wherein this gum solution is used, and whereby printing plates are obtained which exhibit an improved clean-out performance.

qum soln development qumming photopolymer lithog printing plate ST

IT Alcohols, uses

RL: TEM (Technical or engineered material use); USES (Uses)

(amino; gum solution for developing and gumming a photopolymer printing plate.)

ΤТ Alcohols, uses

RL: TEM (Technical or engineered material use); USES (Uses)

(coco, ethoxylated, Lutensol A 8; gum solution for developing and gumming a photopolymer printing plate.)

Polysiloxanes, uses

RL: TEM (Technical or engineered material use); USES (Uses)

(glycidyl group-containing, Edaplan LA 411; gum solution for developing and gumming a photopolymer printing plate.)

Polyvinyl butyrals

RL: TEM (Technical or engineered material use); USES (Uses) (gum solution for developing and gumming a photopolymer printing plate.)

Lithographic plates

(precursor; gum solution for developing and gumming a photopolymer printing plate.)

```
TT
    9004-53-9, Dextrin
     RL: TEM (Technical or engineered material use); USES (Uses)
        (Avedex 37LAC19; gum solution for developing and gumming a photopolymer
       printing plate.)
     691397-13-4, Pluronic PE 9400
     RL: TEM (Technical or engineered material use); USES (Uses)
        (Pluronic PE 10300; gum solution for developing and gumming a photopolymer
       printing plate.)
    64-18-6, Formic acid, uses 64-19-7, Acetic acid, uses
     65-85-0, Benzoic acid, uses 77-92-9, Citric acid, uses 78-96-6,
     1-Amino-2-propanol 87-69-4, Tartaric acid, uses 102-71-6,
     Triethanolamine, uses 104-15-4, p-Toluenesulfonic acid, uses
    N, N-Dimethylamino-ethanol 124-68-5,
     2-Amino-2-methyl-1-propanol 126-92-1, Texapon 842 141-43-5, uses
     149-30-4, 2-Mercaptobenzothiazole 527-07-1, Sodium gluconate 574-93-6,
     Heliogen Blue D 7490 1320-67-8, Dowanol PM 5205-93-6
                                                               7005-47-2,
     2-(N,N-Dimethyl)amino-2-methyl-1-propanol 7189-82-4,
     2,2'-Bis(2-chlorophenyl)-4,4',5,5'-tetraphenyl-1,2'-biimidazole
     7647-01-0, Hydrochloric acid, uses 7664-38-2, Phosphoric acid, uses
     7664-93-9, Sulfuric acid, uses 7697-37-2, Nitric acid, uses 9002-98-6,
     Lupasol P 9003-20-7D, Poly(vinyl acetate), hydrolyzed, cyclic acetal
     with butyraldehyde 26636-37-3, Sapogenat T 130 32509-66-3, Hostanox O
     3 36355-55-2, Mono-Z 1620 41593-38-8, Dowarol PPh 70559-25-0,
     Emulsogen TS 160 73539-65-8, FST 426R 937016-53-0, Acticide LA 1206
     937023-63-7
     RL: TEM (Technical or engineered material use); USES (Uses)
       (gum solution for developing and gumming a photopolymer printing plate.)
RE.CNT 6
             THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD
(1) Az Electronic Materials Usa Co; EP 1650605 A 2006 CAPLUS
(2) Fuji Photo Film Co Ltd; EP 1602982 A 2005 CAPLUS
(3) Fuji Photo Film Co Ltd; EP 1621339 A 2006 CAPLUS
(4) Fuji Photo Film Co Ltd; EP 1755002 A 2007 CAPLUS
(5) Kodak Polychrome Graphics Co; EP 1103859 A 2001 CAPLUS
(6) Williams; WO 2005111727 A 2005 CAPLUS
L9
    ANSWER 6 OF 55 CAPLUS COPYRIGHT 2009 ACS on STN
AN
    2008:1127254 CAPLUS
DN
    149:381792
ED
    Entered STN: 19 Sep 2008
    Aqueous-based insulating fluids and related methods
IN
    Ezell, Ryan; Miller, Jeff; Perez, Greg
PA
SO
    U.S. Pat. Appl. Publ., 9pp.
    CODEN: USXXCO
    Patent
LA
   English
INCL 174030000; 252062000
     51-2 (Fossil Fuels, Derivatives, and Related Products)
     Section cross-reference(s): 38
FAN.CNT 4
     PATENT NO.
                         KIND
                                DATE
                                          APPLICATION NO.
     US 20080223596
                               20080918
                                           US 2007-685923
                         A1
                                                                   20070314
     WO 2008110798
                         A2
                               20080918
                                           WO 2008-GB868
                                                                   20080312
                               20090226
     WO 2008110798
                         A3
         W: AE, AG, AL, AM, AO, AT, AU, AZ, BA, BB, BG, BH, BR, BW, BY, BZ,
            CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DO, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE,
             KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LY, MA, MD,
            ME, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH,
             PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM,
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TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW
         RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HR, HU,
             IE, IS, IT, LT, LU, LV, MC, MT, NL, NO, PL, PT, RO, SE, SI, SK,
             TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD,
             TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW,
             AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AP, EA, EP, OA
PRAT US 2007-685909
                        A
                               20070314
    US 2007-685923
                          Α
                                20070314
CLASS
PATENT NO.
               CLASS PATENT FAMILY CLASSIFICATION CODES
US 20080223596 INCL
                       174030000: 252062000
                IPCI H01B0017-34 [I,A]; H01B0017-00 [I,C*]
                NCL.
                       174/030.000; 252/062.000
WO 2008110798
                IPCI
                       C10M0169-04 [I,A]; C10M0169-00 [I,C*]; C10M0173-02
                       [I,A]; C09K0008-12 [I,A]; C10N0030-08 [I,A];
                       C10N0040-00 [I,A]; C10N0040-08 [I,A]; C10M0173-02
                        [I,C]; C10M0173-02 [I,A]; C09K0008-02 [I,C];
                       C09K0008-12 [I,A]
                 ECLA
                       C10M173/02; C10M177/00; M10M; M10M; M10M; M10M; M10M;
                       M10M; M10M; M10M; M10M; M10M; M10M; M10M; M10M; M10M;
                       M10N; M10N; M10N; M10N; M10N; M10N; M10N
   Provided herein are compas, that include an aqueous-based insulating fluid
     that comprises an aqueous base fluid, a water-miscible organic liquid, and a
     synthetic polymer. In another embodiment, provided herein is a method of
     forming an aqueous-based insulating fluid comprising: mixing an aqueous base
fluid
     and a water-miscible organic liquid to form a mixture; adding at least one
     synthetic polymer to the mixture; allowing the polymer to hydrate;
     optionally adding a crosslinking agent to the mixture comprising the
     synthetic polymer to crosslink the synthetic polymer; placing the mixture
     comprising the synthetic polymer in a chosen location; allowing the mixture
    comprising the synthetic polymer to activate to form a gel therein.
ST
    ag insulating fluid
     Amines, uses
     RL: TEM (Technical or engineered material use); USES (Uses)
        (aliphatic; aqueous-based insulating fluids and related methods)
     Biocides
     Brines
     Buffers
     Corrosion inhibitors
     Gelation agents
     Gels
     Hydration, chemical
     Pipelines
     Surfactants
     Thermal insulators
     Thickening agents
     Tracers
     Waters
    Wells
        (aqueous-based insulating fluids and related methods)
     Acrylic polymers, uses
     Alcohols, uses
     Alditols
     Amines, uses
     Esters, uses
     Glass beads
    Glycols, uses
     Imines
     Phenolic resins, uses
     Phenols, uses
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Polyoxyalkylenes, uses
     RL: TEM (Technical or engineered material use); USES (Uses)
        (aqueous-based insulating fluids and related methods)
     Amines, uses
     RL: TEM (Technical or engineered material use); USES (Uses)
        (aralkyl; aqueous-based insulating fluids and related methods)
     Pipes and Tubes
        (conduits, underground; aqueous-based insulating fluids and related
       methods)
     Glycols, uses
     RL: TEM (Technical or engineered material use); USES (Uses)
        (ethers; aqueous-based insulating fluids and related methods)
IT
     Ethers, uses
     RL: TEM (Technical or engineered material use); USES (Uses)
        (glycol; aqueous-based insulating fluids and related methods)
     Spheres
        (hollow; aqueous-based insulating fluids and related methods)
     Rheology
        (modifiers; aqueous-based insulating fluids and related methods)
ΙT
     Hydration catalysts
       (neg.; aqueous-based insulating fluids and related methods)
        (organic: aqueous-based insulating fluids and related methods)
     Polvamines
     RL: TEM (Technical or engineered material use); USES (Uses)
       (polyalkylene-; aqueous-based insulating fluids and related methods)
     Alcohols, uses
     RL: TEM (Technical or engineered material use); USES (Uses)
       (polyhydric; aqueous-based insulating fluids and related methods)
     Alcohols, uses
     RL: TEM (Technical or engineered material use); USES (Uses)
        (trihydric; aqueous-based insulating fluids and related methods)
     Weight
        (weighting agents; aqueous-based insulating fluids and related methods)
     50-00-0, Formaldehyde, uses 50-78-2, Aspirin 56-81-5, Glycerol, uses
     57-55-6, Propylene glycol, uses 65-45-2, Salicylamide
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                69-72-7, Salicylic acid, uses 74-85-1D, Ethylene, reaction
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    products with ethylene 79-06-1D, Acrylamide, polymers
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     Acrylic acid, esters, polymers 79-20-9, Methyl acetate
    Methacrylic acid, esters, polymers 88-12-0, uses 98-00-0, Furfurvl
             99-76-3, Methyl p-hydroxybenzoate 100-97-0,
     Hexamethylenetetramine, uses 107-21-1, Ethylene glycol, uses 107-22-2,
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              107-31-3, Methyl formate 108-01-0, 2-(
     Dimethylamino)ethanol 108-95-2, Phenol, uses
     109-89-7, Diethylamine, uses
                                   110-65-6, Butyne diol
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     Triethylene glycol 115-77-5, Pentaerythritol, uses 118-55-8, Phenyl
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     123-31-9, Hydroquinone, uses 126-30-7, Neopentyl glycol
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     2-Aminoethanol, uses 141-53-7, Sodium formate 141-78-6,
     Ethyl acetate, uses 150-13-0, p-Aminobenzoic acid
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    carbonate, uses 590-29-4, Potassium formate 591-27-5, m-Aminophenol 1321-11-5, Aminobenzoic acid 3495-36-1, Cesium
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    Sodium chloride, uses 7647-15-6, Sodium bromide (NaBr), uses 7732-18-5, Water, uses 7789-41-5, Calcium bromide (CaBr2)
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     Polyethylenimine 9003-01-4, Acrylic acid polymers 9003-05-8,
    Polyacrylamide 9003-21-8, Poly (methyl acrylate) 9003-49-0, Poly
    (butyl acrylate) 9003-77-4, Poly(2-ethylhexyl acrylate)
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     Poly(methylmethacrylate) 10043-52-4, Calcium chloride, uses
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11070-67-0, Butynediol 12542-32-4, Butenediol 15214-89-8D, derivs.,
               24621-17-8, Zirconium bromide (ZrBr2) 24800-44-0,
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    25265-71-8, Dipropylene glycol 25265-75-2, Butanediol 25322-68-3,
    Polyethylene glycol 25322-69-4 26124-23-2.
    Acrylamide-n-vinylpyrrolidone copolymer 27119-07-9 29348-79-6,
    Pentanediol
                 40623-75-4
    RL: TEM (Technical or engineered material use); USES (Uses)
        (aqueous-based insulating fluids and related methods)
    ANSWER 7 OF 55 CAPLUS COPYRIGHT 2009 ACS on STN
AN
    2008:644143 CAPLUS
    149:179843
    Entered STN: 30 May 2008
    Controlled generation of hydrogen from formic acid amine adducts
    at room temperature and application in H2/O2 fuel cells
    Loges, Bjoern; Boddien, Albert; Junge, Henrik; Beller, Matthias
    Leibniz-Institut fuer Katalyse e.V., Universitaet Rostock, Rostock, 18059,
    Germany
    Angewandte Chemie, International Edition (2008), 47(21), 3962-3965
    CODEN: ACIEF5; ISSN: 1433-7851
    Wiley-VCH Verlag GmbH & Co. KGaA
    Journal
    English
    52-1 (Electrochemical, Radiational, and Thermal Energy Technology)
    Section cross-reference(s): 67
    Hydrogen is generated from formic acid amine adducts at room
    temperature used directly in fuel cells (see picture for apparatus). Ruthenium
    phosphine systems act as catalysts in this transformation.
    controlled hydrogen formic acid amine adduct ruthenium catalysis
    Controlled atmospheres
    Decomposition
    Decomposition catalysts
        (controlled generation of hydrogen from formic acid amine
       adducts at room temperature and application in H2/O2 fuel cells)
    Organometallic compounds
    RL: CAT (Catalyst use); USES (Uses)
        (controlled generation of hydrogen from formic acid amine
       adducts at room temperature and application in H2/O2 fuel cells)
    Amines, reactions
    RL: RCT (Reactant); RACT (Reactant or reagent)
        (controlled generation of hydrogen from formic acid amine
       adducts at room temperature and application in H2/O2 fuel cells)
    Fuel cells
        (fuel for; controlled generation of hydrogen from formic acid
       amine adducts at room temperature and application in H2/O2 fuel cells)
    Carbon black, uses
    RL: CAT (Catalyst use); USES (Uses)
        (support; controlled generation of hydrogen from formic acid
       amine adducts at room temperature and application in H2/02 fuel cells)
    1333-74-0P, Hydrogen, preparation
    RL: ANT (Analyte); SPN (Synthetic preparation); ANST (Analytical study);
    PREP (Preparation)
        (controlled generation of hydrogen from formic acid amine
       adducts at room temperature and application in H2/O2 fuel cells)
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    trichloride
                  10049-08-8, Ruthenium trichloride 12078-28-3, Dicarbonyl
    cyclopentadienyl-iodoiron 15529-49-4, Dichlorotris(triphenylphosphine)
    ruthenium
               52462-29-0, Bis(dichloro(p-cymene)ruthenium)
    RL: CAT (Catalyst use); USES (Uses)
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(controlled generation of hydrogen from formic acid amine adducts at room temperature and application in H2/O2 fuel cells)

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1309-37-1P, Ferric oxide, uses
                                     1040186-00-2P
     RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation);
     USES (Uses)
        (controlled generation of hydrogen from formic acid amine
        adducts at room temperature and application in H2/O2 fuel cells)
     630-08-0, Carbon monoxide, formation (nonpreparative)
     RL: FMU (Formation, unclassified); FORM (Formation, nonpreparative)
        (controlled generation of hydrogen from formic acid amine
        adducts at room temperature and application in H2/O2 fuel cells)
     7440-37-1, Argon, uses
     RL: NUU (Other use, unclassified); USES (Uses)
        (controlled generation of hydrogen from formic acid amine
        adducts at room temperature and application in H2/O2 fuel cells)
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     108-01-0, Dimethylaminoethanol
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                        4385-04-0 7378-99-6, Dimethyloctylamine
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     7664-41-7, Ammonia, reactions
                                     15077-13-1, Formic acid, compound
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     RL: RCT (Reactant); RACT (Reactant or reagent)
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        adducts at room temperature and application in H2/02 fuel cells)
     68-12-2, Dimethylformamide, uses
     RL: NUU (Other use, unclassified); USES (Uses)
        (solvent effects; controlled generation of hydrogen from formic
        acid amine adducts at room temperature and application in H2/O2 fuel cells)
RE.CNT
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- DN
- 147:228569
- ED Entered STN: 30 Jul 2007
- ΤТ Identification of the Structural Requirements for Mutagenicity, by Incorporating Molecular Flexibility and Metabolic Activation of Chemicals. II. General Ames Mutagenicity Model. [Erratum to document cited in CA146:516278]
- AU Serafimova, R.; Todorov, M.; Pavlov, T.; Kotov, S.; Jacob, E.; Aptula, A.; Mekenvan, O.
- CS Laboratory of Mathematical Chemistry, University Prof. As. Zlatarov, Bourga, 8000, Bulg.
- SO Chemical Research in Toxicology (2007), 20(8), 1225 CODEN: CRTOEC; ISSN: 0893-228X
- American Chemical Society PB
- DT Journal
- LA English
- 4-6 (Toxicology)
- AB On page 673, in the conclusion section, the text, "As a comparative exercise, the alerts used in the present work were compared with three alert lists of Ashby, Kazius, and Benigni, " should read: "As a comparative exercise, the alerts used in the present work were compared with alert lists of Ashby and Kazius, as well as the lists reported by Benigni in his review.".
- ST erratum mutagenicity mol flexibility QSAR model mutagen
- ΙT Molecular topology
 - Mutagenicity
 - Mutagens
 - Salmonella typhimurium
 - Simulation and Modeling
 - (identification of structural requirements for mutagenicity, by incorporating mol. flexibility and metabolic activation of chems. in general Ames mutagenicity model (Erratum)) Polyoxyalkylenes, biological studies
- RL: ADV (Adverse effect, including toxicity); PRP (Properties); BIOL (Biological study) (identification of structural requirements for mutagenicity, by
 - incorporating mol. flexibility and metabolic activation of chems. in general Ames mutagenicity model (Erratum))
 - Structure-activity relationship
 - (mutagenic; identification of structural requirements for mutagenicity, by incorporating mol. flexibility and metabolic activation of chems. in general Ames mutagenicity model (Erratum))
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RL: ADV (Adverse effect, including toxicity); PRP (Properties); BIOL
(Biological study)
   (identification of structural requirements for mutagenicity, by
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Glycidaldehyde 768-52-5, N-Isopropylaniline 785-30-8, 4,4'-Diaminobenzanilide 793-24-8 828-00-2, Dimethoxane 834-28-6, Phenformin hydrochloride 839-90-7 842-07-9, Solvent yellow 14 872-50-4, N-Methyl-2-pyrrolidinone, biological studies 874-42-0, 2,4-Dichlorobenzaldehyde 879-39-0 881-03-8, I-Nitro-2-methylnaphthalene 920-66-1 924-42-5, N-Methylolacrylamide RL: ADV (Adverse effect, including toxicity); PRP (Properties); BIOL (Biological study)

incorporating mol. flexibility and metabolic activation of chems. in general Ames mutagenicity model (Erratum)) 931-97-5, Cyclohexanone cyanohydrin 933-75-5, 2,3,6-Trichlorophenol 933-78-8, 2,3,5-Trichlorophenol 934-32-7, 2-Aminobenzimidazole 935-95-5, 2,3,5,6-Tetrachlorophenol 952-21-6, 3-Methyl-4'-nitrobiphenyl 958-93-0, Thenyldiamine hydrochloride 968-81-0, Acetohexamide 982-57-0, biological studies 989-38-8, Basic red 1 992-59-6, Direct red 2 999-55-3, Allyl acrylate 999-81-5 1025-15-6, Triallyl isocyanurate 1034-41-9, Chlordecone alcohol 1071-83-6, Glyphosate 1072-52-2, 1-Aziridineethanol 1116-40-1, Triisobutylamine 1116-54-7, N-Nitrosodiethanolamine 1122-54-9, 4-Acetylpyridine 1126-61-0 1143-38-0, 1,8-Dihydroxyanthrone 1163-19-5, Decabromodiphenyl ether 1187-42-4, Diaminomaleonitrile 1212-29-9, N.N'-Dicyclohexylthiourea 1229-35-2, Methdilazine hydrochloride 1241-94-7, biological studies 1465-25-4 1467-79-4, Dimethyl cyanamide 1484-12-4, 9-Methylcarbazole 1504-74-1, o-Methoxycinnamaldehyde 1522-92-5, 3-Bromo-2,2-bis(bromomethyl)propanol 1562-94-3, p-Azoxvanisole 1570-64-5, p-Chloro-o-cresol 1571-08-0, Methyl p-formylbenzoate 1576-35-8, p-Toluenesulfonyl hydrazide 1596-84-5, biological studies 1606-67-3, 1-Pyrenamine 1634-78-2 1635-61-6, 5-Chloro-2-nitroaniline 1646-75-9, Aldicarb oxime 1675-54-3 1694-09-3, Acid violet 49 1694-20-8, (E)-4-Nitrostilbene 1758-68-5, 1,2-Diaminoanthraquinone 1761-71-3 1777-84-0, 3-Nitro-p-acetophenetide 1806-54-8 1817-73-8, 2-Bromo-4,6-dinitroaniline 1825-21-4, Pentachloroanisole 1836-75-5, Nitrofen 1854-26-8, Dimethyloldihydroxyethyleneurea 1897-45-6 1912-24-9, Atrazine 1918-02-1, Picloram 1929-82-4 1934-21-0, Acid yellow 23 1936-15-8, Acid orange 10 1937-37-7, Direct black 38 1948-33-0, tert-Butylhydroguinone 1955-45-9, Pivalolactone 1972-08-3, trans-A9-Tetrahydrocannabinol 2016-88-8, Amiloride hydrochloride 2039-87-4, o-Chlorostyrene 2045-52-5, Phenbenzamine hydrochloride 2050-92-2, Di-N-amylamine 2052-07-5, 2-Bromobiphenyl 2107-76-8 2113-57-7, 3-Bromobiphenyl 2143-88-6, 4-Methyl-4'-nitrobiphenyl 2150-54-1, Direct blue 25 2150-60-9 2157-01-9, n-Octyl methacrylate 2164-17-2, Fluometuron 2179-59-1, Allyl propyl disulfide 2185-92-4, 2-Biphenylamine hydrochloride 2206-89-5, 2-Chloroethyl acrylate 2210-28-8, n-Propvl methacrylate 2213-63-0, 2,3-Dichloroquinoxaline 2243-61-0, 1,4-Naphthalenediamine 2243-62-1, 1,5-Naphthalenediamine 2244-16-8, D-Carvone 2244-21-5, Potassium dichlorocyanurate 2385-85-5, Mirex 2425-85-6, C.I. Pigment red 3 2429-71-2, Direct blue 8 2429-73-4 2429-74-5, Direct blue 15 2429-80-3, C. I. Acid orange 45 2432-99-7, 11-Aminoundecanoic acid 2438-88-2 2439-35-2, biological studies 2461-15-6, 2-Ethylhexyl glycidyl ether 2465-27-2, Basic yellow 2475-45-8, 1,4,5,8-Tetraaminoanthraquinone 2493-84-7, p-Octyloxybenzoic acid 2508-20-5, 2-Nitrosofluorene 2528-36-1, Dibutyl phenyl phosphate 2602-46-2, Direct blue 6 2645-07-0, 4-Nitrohippuric acid 2646-17-5 2675-77-6, Chloroneb 2682-20-4, 2-Methyl-4-Isothiazolin-3-one 2698-41-1, o-Chlorobenzalmalononitrile 2735-04-8, 2,4-Dimethoxyaniline 2782-57-2, Dichloroisocyanuric acid 2782-91-4, Tetramethylthiourea 2783-94-0, FD&C yellow 6 2784-94-3, HC blue 1 2810-69-7 2832-40-8, Disperse yellow 3 2835-95-2, 3-Amino-6-methylphenol 2871-01-4, HC Red 3 2873-97-4, Diacetone

acrylamide 2893-78-9, Sodium dichlorocyanurate 2941-64-2, S-Ethyl chlorothiocarbonate 2945-96-2, C. I. Direct black 17 3018-12-0, 3025-77-2 3066-70-4, biological studies Dichloroacetonitrile 3068-88-0, β-Butyrolactone 3081-14-9 3129-91-7, Dicyclohexylamine nitrite 3160-37-0, Piperonylidene acetone 3165-93-3, 4-Chloro-o-toluidine hydrochloride 3179-47-3, n-Decyl methacrylate 3209-22-1, 2,3-Dichloronitrobenzene 3237-50-1, Alloxan monohydrate 3252-43-5, Dibromoacetonitrile 3266-23-7, 2,3-Epoxybutane Octachlorodibenzo-p-dioxin 3319-31-1 3322-93-8 3333-52-6, Tetramethylsuccinonitrile 3468-63-1, Pigment grange 5 3524-68-3, Pentaerythritol triacrylate 3544-23-8 3546-10-9, biological studies 3567-69-9, Acid red 14 3626-28-6, Direct green 1 3648-20-2, Diundecyl phthalate 3658-77-3, 2,5-Dimethyl-4-hydroxy-3(2H)-furanone 3682-19-7 3688-53-7 3689-24-5 3731-39-3 3761-53-3, Acid red 26 4067-16-7, Pentaethylenehexamine 4080-31-3 4098-71-9, Isophorone diisocyanate 4170-30-3, Crotonaldehyde 4196-86-5 4196-87-6 4198-19-0 4309-66-4, trans-4-Aminostilbene 4337-65-9, Mono(2-ethylhexyl) adipate 4342-03-4, Dacarbazine 4345-03-3 4350-09-8, 5-HydroxyL-tryptophan 4403-61-6, 2-Methyl-2-butenenitrile 4418-26-2, Sodium dehydroacetate 4424-06-0, Pigment orange 43 4444-68-2 4460-86-0, 2,4,5-Trimethoxybenzaldehyde 4465-94-5 4548-53-2, FD&C red 4 4553-62-2, α-Methyl glutaronitrile 4568-28-9, Triethanolamine stearate 4635-87-4, 3-Pentenenitrile 4637-56-3 4655-34-9, Isopropyl methacrylate 4719-04-4 4801-39-2, 2-Aminoacetanilide hydrochloride 4802-20-4, Limonene dimercaptan 4823-47-6, 2-Bromoethyl acrylate 4901-51-3. 2,3,4,5-Tetrachlorophenol 5064-31-3, Nitrilotriacetic acid trisodium salt 5131-58-8, 4-Nitro-m-phenylenediamine 5131-60-2, 4-Chloro-m-phenylenediamine 5160-02-1, D And C red 9 5216-25-1, 4-Chlorobenzotrichloride 5307-14-2 5323-95-5, Sodium ricinoleate 5397-31-9 5466-77-3 5466-84-2, 4-Nitrophthalic anhydride 5493-45-8 5989-27-5, D-Limonene 6041-94-7, C.I. Pigment red 2 6088-51-3 6109-97-3, 3-Amino-9-ethylcarbazole monohydrochloride 6112-76-1, 6-Mercaptopurine monohydrate 6197-30-4 6201-87-2, 5-Amino-3-sulfosalicylic acid 6219-89-2 6285-57-0, 2-Amino-6-nitrobenzothiazole 6287-38-3, 3,4-Dichlorobenzaldehyde 6317-18-6, biological studies 6358-07-2, 2-Amino-4-chloro-5-nitrophenol 6358-23-2 6358-29-8, Direct red 39 6358-31-2, C.I. Pigment yellow 74 6358-53-8, Solvent red 80 6358-85-6, Pigment yellow 12 6369-59-1 6373-74-6, Acid orange 3 6428-94-0, Direct violet 32 6459-94-5, Acid red 114 6471-49-4, Pigment red 23 6483-86-9 6533-68-2, Scopolamine hydrobromide trihydrate 6610-08-8, 2-Nitrosonaphthalene 6810-26-0 6959-47-3, 2-(Chloromethyl)pyridine hydrochloride 6959-48-4, 3-(Chloromethyl)pyridine hydrochloride 7149-26-0, Linalyl anthranilate 7166-19-0, β-Bromo-β-nitrostyrene 7177-48-2, Ampicillin trihydrate 7195-43-9, Isophthalic acid diglycidyl ester 2-Phenyl-2-ethylmalondiamide 7314-08-1 7493-63-2, Allyl anthranilate 7756-96-9, Butyl anthranilate 7779-16-0, Cyclohexyl anthranilate 7779-77-3, Isobutyl anthranilate 8003-22-3, Solvent vellow 33 10043-35-3, Boric acid (H3BO3), biological studies 10125-76-5, 4-Nitrosobiphenyl 10143-23-4, 2,3-Dimethyl-1-pentanol 10213-75-9 10277-43-7, Lanthanum nitrate hexahydrate 10318-26-0, Dibromodulcitol RL: ADV (Adverse effect, including toxicity); PRP (Properties); BIOL (Biological study)

(identification of structural requirements for mutagenicity, by incorporating mol. flexibility and metabolic activation of chems. in general Ames mutagenicity model (Erratum))

T 10605-21-7, Carbendazim 11097-69-1, PCB 1254 12224-98-5, Pigment red 81 12225-21-7, Pigment yellow 100 12789-03-6, Chlordane 13014-18-1 13014-24-9 13048-33-4, 1,6-Hexanediol diacrylate 13071-79-9, biological studies 13098-39-0 13114-72-2 13284-42-9, 2-Pentenenitrile 13360-63-9, Ethyl N-butylamine 13366-73-9, Photodieldrin 13552-21-1 13552-44-8, 4,4'-Methylenedianiline

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dihydrochloride 13674-84-5 13674-87-8 13684-63-4, Phenmedipham
13889-92-4, Propyl chlorothioformate 13952-84-6, sec-Butylamine
13961-86-9, biological studies 14371-10-9, trans-Cinnamaldehyde
14882-18-9, Bismuth subsalicylate 14901-07-6 15110-74-4,
                                                           15481-70-6
2,5-Dinitrofluorene 15121-84-3, o-Nitrophenethylalcohol
15893-52-4 15950-66-0, 2,3,4-Trichlorophenol 16219-75-3, Ethylidene
           16238-56-5 16452-01-0 16529-56-9,
norbornene
2-Methyl-3-butenenitrile 17026-81-2, 3-Amino-4-ethoxyacetanilide
17341-40-1 17359-54-5 17369-59-4, 3-Propylidenephthalide 17372-87-1,
Eosin 17433-31-7 17804-35-2, Benomyl 17831-71-9, Tetraethylene
glycol diacrylate
                  17924-92-4, Zearalenone 18024-11-8,
1,4,9-Trimethylcarbazole 18028-55-2, 1,4-Dimethylcarbazole 18028-56-3,
1,4,6-Trimethylcarbazole 18662-53-8, Nitrilotriacetic acid trisodium
salt monohydrate 19315-64-1 19660-16-3, 2,3-Dibromopropyl acrylate
19686-73-8, 1-Bromo-2-propanol 19780-11-1 20020-02-4,
1,2,3,4-Tetrachloronaphthalene 20265-97-8, p-Anisidine hydrochloride 20548-62-3, biological studies 20702-77-6, Neohesperidin dihydrochalcone
21285-46-1, trans-2,3-Dibromo-2-butene-1,4-diol 21739-91-3, Cytembena
21829-25-4, Nifedipine 22224-92-6, Phenamiphos
                                                  23255-93-8, Hycanthone
methanesulfonate 23564-05-8, Thiophanate methyl 24140-30-5
24169-02-6, Econazole nitrate 24325-70-0,
trans-4-Methyl-4'-nitrostilbene 24370-25-0, 2-Benzimidazolylurea 24382-04-5, Propanedial sodium 24554-26-5,
N-[4-(5-Nitro-2-furvl)-2-thiazolvl]formamide
                                              24815-24-5, Rescinnamine
25322-68-3, Peg 25637-99-4, Hexabromocyclododecane 25843-45-2,
              25953-06-4 26446-35-5, Acetin 26471-62-5
Azoxymethane
Kathon 893 26638-28-8, Methyl pentachlorostearate 26761-40-0,
Diisodecvl phthalate 28322-02-3, 4-Acetvlaminofluorene 29385-43-1,
Tolyltriazole 29743-15-5, 4-Butyloxybenzal-4'-ethylaniline 29761-21-5,
Isodecyl diphenyl phosphate 29964-84-9, Isodecyl methacrylate
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33229-34-4, HC blue 2 34807-41-5, Mezerein 36355-01-8,
Hexabromobiphenyl 37853-59-1 38848-76-9 39156-41-7,
2,4-Diaminoanisole sulfate 41122-70-7 42397-64-8, 1,6-Dinitropyrene
42397-65-9, 1,8-Dinitropyrene 52551-67-4 54810-82-1,
3,5-Dimethyl-4-aminobiphenyl 54827-17-7, 3,3',5,5'-Tetramethylbenzidine
56803-37-3, tert-Butylphenyl diphenyl phosphate 62625-14-3,
2-Amino-6-chloro-4-nitrophenol hydrochloride 64532-97-4, biological
        67219-70-9, 1-Butyl-2-aminonaphthalene 69314-47-2,
3-Methyl-4-nitrobiphenyl
                         69884-05-5 70634-28-5 72917-35-2,
1,4-Dimethyl-6-hydroxy-3-nitrocarbazole 74518-95-9
76002-91-0 78491-02-8, Diazolidinylurea 92814-28-3,
4-Ethyl-3-nitrobiphenyl 108100-28-3, 2-Methyl-7-nitrofluorene
126335-31-7 126335-36-2 127502-68-5, 2-Isopropyl-4-phenylnitrobenzene
127502-69-6, 3-Isopropyl-4-aminobiphenyl 127750-13-4 128714-75-0,
1,6-Dinitrobenzo[a]pyrene 128714-76-1, 3,6-Dinitrobenzo[a]pyrene
129117-54-0, 1,4-Dimethyl-6-methoxy-3-aminocarbazole 188107-70-2,
9-Methvl-2-nitro-9H-carbazole 188107-72-4,
                                      189084-64-8 275795-12-5
1.4.6-Trimethvl-3-nitro-9H-carbazole
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            279242-14-7 279242-16-9 279242-17-0 314084-63-4,
279242-12-5
3,5-Diethyl-4-aminobiphenyl 345667-01-8 345667-02-9 345667-57-4
345667-58-5 345667-59-6 345667-60-9 345667-61-0 345667-62-1 389104-53-4, 1-Ethyl-2-aminonaphthalene 389104-54-5 389104-55-6,
1-tert-Butyl-2-aminonaphthalene 389104-56-7, 1-Ethyl-2-aminofluorene
389104-57-8, 1-Isopropyl-2-aminofluorene 389104-58-9,
1-Butyl-2-aminofluorene 389104-59-0, 1-tert-Butyl-2-aminofluorene
389104-60-3, 3-Ethyl-4-aminobiphenyl 389104-61-4, 3-Butyl-4-aminobiphenyl 389104-62-5, 3,5-Diisopropyl-4-aminobiphenyl
RL: ADV (Adverse effect, including toxicity); PRP (Properties); BIOL
(Biological study)
   (identification of structural requirements for mutagenicity, by
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incorporating mol. flexibility and metabolic activation of chems. in general Ames mutagenicity model (Erratum))

- ANSWER 9 OF 55 CAPLUS COPYRIGHT 2009 ACS on STN 1.9
- AN 2007:334667 CAPLUS
- DN 146:516278
- Entered STN: 25 Mar 2007
- Identification of the Structural Requirements for Mutagenicity, by Incorporating Molecular Flexibility and Metabolic Activation of Chemicals. II. General Ames Mutagenicity Model
- ΑU Serafimova, R.; Todorov, M.; Pavlov, T.; Kotov, S.; Jacob, E.; Aptula, A.; Mekenyan, O.
- CS Laboratory of Mathematical Chemistry, University Prof. As. Zlatarov, Bourgas, 8000, Bulg. SO
- Chemical Research in Toxicology (2007), 20(4), 662-676 CODEN: CRTOEC; ISSN: 0893-228X
- PB American Chemical Society
- DT Journal LA English
- CC
- 4-6 (Toxicology)
 - The tissue metabolic simulator (TIMES) modeling approach is a hybrid expert system that couples a metabolic simulator together with structure toxicity rules, underpinned by structural alerts, to predict interaction of chems. or their metabolites with target macromols. Some of the structural alerts representing the reactivity pattern-causing effect could interact directly with the target whereas others necessitated a combination with two- or three-dimensional quant. structure-activity relationship models describing the firing of the alerts from the rest of the mols. Recently, TIMES has been used to model bacterial mutagenicity (O. Mekenyan, O., et al., 2004). The original model was derived for a single tester strain, Salmonella typhimurium (TA100), using the Ames test by the National Toxicol. Program (NTP). The model correctly identified 82% of the primary acting mutagens, 94% of the nonmutagens, and 77% of the metabolically activated chems. in a training set. The identified high correlation between activities across different strains changed the initial strategic direction to look at the other strains in the next modeling developments. In this respect, the focus of the present work was to build a general mutagenicity model predicting mutagenicity with respect to any of the Ames tester strains. The use of all reactivity alerts in the model was justified by their interaction mechanisms with DNA, found in the literature. The alerts identified for the current model were analyzed by comparison with other established alerts derived from human experts. In the new model, the original NTP training set with 1341 structures was expanded by 1626 proprietary chems. provided by BASF AG. Eventually, the training set consisted of 435 chems., which are mutagenic as parents, 397 chems, that are mutagenic after S9 metabolic activation, and 2012 nonmutagenic chems. The general mutagenicity model was found to have 82% sensitivity, 89% specificity, and 88% concordance for training set chems. The model applicability domain was introduced accounting for similarity (structural, mechanistic, etc.) between predicted chems. and training set chems. for which the model performs correctly.
- mutagenicity mol flexibility QSAR model mutagen
- Molecular topology
- Mutagenicity
 - Mutagens
 - Salmonella typhimurium
 - Simulation and Modeling
 - (identification of structural requirements for mutagenicity, by incorporating mol. flexibility and metabolic activation of chems. in general Ames mutagenicity model)
- Polyoxyalkylenes, biological studies
- RL: ADV (Adverse effect, including toxicity); PRP (Properties); BIOL

(Biological study)

(identification of structural requirements for mutagenicity, by incorporating mol. flexibility and metabolic activation of chems. in general Ames mutagenicity model)

IT Structure-activity relationship

(mutagenic; identification of structural requirements for mutagenicity, by incorporating mol. flexibility and metabolic activation of chems. in general Ames mutagenicity model)

50-00-0, Formaldehyde, biological studies 50-18-0, Cyclophosphamide IT 50-29-3, 4,4'-DDT, biological studies 50-32-8, 3,4-Benzopyrene, biological studies 50-33-9, Phenylbutazone, biological studies 50-34-0, Propantheline bromide 50-53-3, Chlorpromazine, biological studies 50-55-5, Reserpine 50-78-2, Acetylsalicylic acid 50-81-7, Vitamin C, biological studies 51-17-2, Benzimidazole 51-21-8, Fluorouracil 51-28-5, 2,4-Dinitrophenol, biological studies 51-30-9, Isoproterenol hydrochloride 51-41-2 51-43-4, Epinephrine 51-65-0, 4-Fluoro-DL-phenylalanine 51-79-6, Urethane 52-24-4 52-28-8, Codeine phosphate 52-68-6, Trichlorfon 53-03-2, Prednisone 53-19-0 53-70-3, Dibenz[a,h]anthracene 53-86-1, Indomethacin 53-94-1 53-96-3, 2-Acetylaminofluorene 54-31-9, Furosemide 55-18-5, 53-95-2 N-Nitrosodiethylamine 55-21-0, Benzamide 55-38-9, Fenthion 55-86-7, Nitrogen mustard hydrochloride 55-98-1, Myleran 56-04-2, 6-Methyl-2-thiouracil 56-18-8 56-23-5, Carbon tetrachloride, biological studies 56-38-2, Parathion 56-40-6, Glycine, biological studies 56-49-5, 3-Methylcholanthrene 56-53-1 56-54-2, Quinidine 56-57-5, 4-Nitroquinoline-1-oxide 56-72-4, Coumaphos 56-81-5, Glycerol, biological studies 56-93-9 57-13-6, Urea, biological studies 57-14-7, 1,1-Dimethylhydrazine 57-41-0, 5,5-Diphenylhydantoin 57-50-1, Sucrose, biological studies 57-55-6, Propylene glycol, biological studies 57-57-8, β-Propiolactone 57-63-6, Ethynylestradiol 57-66-9, Probenecid 57-68-1, Sulfamethazine 57-71-6 57-74-9 57-83-0, Progesterone, biological studies 57-97-6, 7,12-Dimethylbenz[a]anthracene 58-08-2, Caffeine, biological studies 58-14-0, Pyrimethamine 58-33-3, Promethazine hydrochloride 58-54-8, Ethacrynic acid 58-55-9, Theophylline, biological studies 58-89-9, Lindane 58-90-2, 2,3,4,6-Tetrachlorophenol 58-93-5, Hydrochlorothiazide 58-94-6, Chlorothiazide 59-50-7, p-Chloro-m-cresol 59-87-0, Nitrofurazone 59-89-2, N-Nitrosomorpholine 60-09-3, Solvent yellow 1 60-33-3, Linoleic acid, biological studies 60-34-4, Methylhydrazine 60-35-5, Acetamide, biological studies 60-51-5, Dimethoate 60-57-1, Dieldrin 61-25-6, Papaverine hydrochloride 61-76-7, Phenylephrine hydrochloride 61-82-5, 1H-1, 2, 4-Triazol-3-amine 62-23-7, p-Nitrobenzoic acid 62-44-2, Phenacetin 62-50-0, Ethyl methanesulfonate 62-53-3, Aniline, biological studies 62-55-5, Thioacetamide 62-56-6, Thiourea, biological studies 62-73-7, Dichlorvos 62-75-9, N-Nitrosodimethylamine 63-56-9, Thonzylamine hydrochloride 63-74-1, Sulfanilamide 63-92-3, Phenoxybenzamine hydrochloride 64-18-6, Formic acid, biological studies 64-19-7, Acetic acid, biological studies 64-67-5, Diethyl sulfate 64-75-5, Tetracycline hydrochloride 64-77-7, Tolbutamide 64-86-8, Colchicine 65-45-2, Salicylamide 65-85-0, Benzoic acid, biological studies 66-27-3, Methyl methanesulfonate 66-71-7, o-Phenanthroline 66-75-1, Uracil mustard 66-81-9, Cycloheximide 67-20-9 67-21-0, DL-Ethionine 67-48-1, Choline chloride 67-63-0, Isopropanol, biological studies 67-64-1, Acetone, biological studies 67-72-1, Hexachloroethane 67-97-0, Vitamin D3 68-12-2, N,N-Dimethylformamide, biological studies 69-05-6, Quinacrine dihydrochloride 69-65-8, D-Mannitol 69-74-9, Cytarabine hydrochloride 70-25-7 70-30-4, Hexachlorophene 70-34-8, 1-Fluoro-2, 4-dinitrobenzene 71-58-9, Medroxyprogesterone acetate 72-14-0, Sulfathiazole 72-20-8, Endrin 72-43-5, Methoxychlor 72-54-8, DDD 72-55-9, DDE, biological studies 72-56-0 73-22-3, L-Tryptophan, biological studies 73-49-4,

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Quinethazone 74-11-3, p-Chlorobenzoic acid 74-31-7,
N,N'Diphenyl-p-phenylenediamine 74-85-1, Ethylene, biological studies
74-89-5, Monomethylamine, biological studies 74-96-4, Ethyl bromide 75-00-3, Ethyl chloride 75-04-7, Ethylamine, biological studies
75-05-8, Acetonitrile, biological studies 75-07-0, Acetaldehyde,
biological studies 75-12-7, Formamide, biological studies
Tribromomethane 75-26-3, 2-Bromopropane 75-27-4, Dichlorobromomethane
75-31-0, Isopropylamine, biological studies 75-34-3, 1,1-Dichloroethane
75-35-4, Vinvlidene chloride, biological studies 75-36-5, Acetyl
chloride 75-47-8, Triiodomethane 75-52-5, Nitromethane, biological
studies 75-55-8, Propylenimine 75-64-9, tert-Butylamine, biological
studies 75-65-0, tert-Butyl alcohol, biological studies 75-69-4,
Trichlorofluoromethane 75-83-2, 2,2-Dimethylbutane 75-86-5,
2-Hydroxy-2-methylpropanenitrile 75-87-6, Anhydrous chloral
tert-Butyl hydroperoxide 76-01-7, Pentachloroethane 76-06-2,
Chloropicrin 76-38-0, Methoxyflurane 76-44-8, Heptachlor 77-06-5,
Gibberellic acid 77-47-4, Hexachlorocyclopentadiene 77-65-6,
Bromodiethylacetylcarbamide 77-73-6, Dicyclopentadiene 77-79-2,
3-Sulfolene 78-11-5 78-34-2, Dioxathion 78-38-6, Diethyl
                 78-40-0, Triethyl phosphate 78-42-2,
ethylphosphonate
Tris(2-ethylhexyl) phosphate 78-44-4, Carisoprodol 78-51-3 78-59-1, Isophorone 78-79-5, Isoprene, biological studies 78-81-9, Isobutyl
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RL: ADV (Adverse effect, including toxicity); PRP (Properties); BIOL
(Biological study)
   (identification of structural requirements for mutagenicity, by
   incorporating mol. flexibility and metabolic activation of chems. in
   general Ames mutagenicity model)
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(identification of structural requirements for mutagenicity, by incorporating mol. flexibility and metabolic activation of chems. in general Ames mutagenicity model)

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    RL: ADV (Adverse effect, including toxicity); PRP (Properties); BIOL
     (Biological study)
        (identification of structural requirements for mutagenicity, by
        incorporating mol. flexibility and metabolic activation of chems. in
        general Ames mutagenicity model)
RE.CNT
             THERE ARE 81 CITED REFERENCES AVAILABLE FOR THIS RECORD
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- L9 ANSWER 10 OF 55 CAPLUS COPYRIGHT 2009 ACS on STN
- AN 2006:977103 CAPLUS
- DN 145:356920
- ED Entered STN: 21 Sep 2006
- TI Preparation of hydroxymethylboron derivatives for hydroxymethylation or alkoxymethylation of aromatic rings
 - N Tanaka, Keigo; Inoue, Satoshi; Ito, Daisuke; Murai, Norio; Kaburagi, Yosuke; Shirotori, Shuji; Suzuki, Shuichi; Ohashi, Yoshiaki
- PA Eisai R & D Management Co., Ltd., Japan
- SO PCT Int. Appl., 92pp.
- CODEN: PIXXD2
- DT Patent
- LA Japanese
- CC 29-4 (Organometallic and Organometalloidal Compounds)
- Section cross-reference(s): 21, 25

E MIN	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE		
PT	WO 2006098270	A1	20060921	WO 2006-JP304894	20060313		

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W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH,
            CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,
            GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR,
            KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX,
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                                        EP 2006-715617
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                             20081217 JP 2007-508123
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    IN 2007CN04533
                             20080125
                                        IN 2007-CN4533
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                             20050314
    JP 2005-294589
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    WO 2006-JP304894
                             20060313
CLASS
               CLASS PATENT FAMILY CLASSIFICATION CODES
PATENT NO.
WO 2006098270
               IPCI C07F0005-02 [I,A]; C07F0005-00 [I,C*]
                IPCR C07F0005-00 [I,C]; C07F0005-02 [I,A]
               ECLA
                     C07F005/02
EP 1867650
               IPCI C07F0005-02 [I,A]; C07F0005-00 [I,C*]
               IPCR C07F0005-00 [I,C]; C07F0005-02 [I,A]
               ECLA C07F005/02
JP 4198742
               IPCI C07F0005-02 [I,A]; C07F0005-00 [I,C*]
US 20080242859 IPCI C07F0005-02 [I,A]; C07F0005-00 [I,C*]
               NCL
                      544/069.000; 544/229.000; 546/013.000; 548/405.000;
                      549/213.000; 560/122.000; 560/125.000; 564/008.000;
                      568/006.000
OS
    MARPAT 145:356920
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AB This document discloses boron compds. or salts or solvates thereof for the hydroxymethylation and alkoxymethylation of aromatic rings. For example, claimed are compds. represented by XOCH2BF3M [M = alkali metal, etc.; X = (un) substituted alkyl, (un) substituted cycloalkyl, (un) substituted non-aromatic heterocyclic ring, etc.]. Thus, potassium methoxymethyl trifluoroborate (I) was prepared in 2 steps from tributyltin hydride and chloromethyl Me ether. I was used in the preparation of 1-methoxymethyl-4-nitrobenzene from 4-nitrophenyl

trifluoromethanesulfonate.

hydroxymethylboron deriv prepn arom ring hydroxymethylation alkoxymethylation; methoxymethylnitrobenzene prepn; nitrophenyl trifluoromethanesulfonate reaction potassium methoxymethyl trifluoroborate Methylation

(alkoxy-; preparation of hydroxymethylboron derivs. for hydroxymethylation or alkoxymethylation of aromatic rings)

Hydroxymethylation

(preparation of hydroxymethylboron derivs, for hydroxymethylation or alkoxymethylation of aromatic rings)

Aromatic compounds

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of hydroxymethylboron derivs. for hydroxymethylation or alkoxymethylation of aromatic rings)

67-63-0, 2-Propanol, reactions 71-36-3, 1-Butanol, reactions 74-88-4, Iodomethane, reactions 74-95-3, Dibromomethane 75-98-9, Pivalic acid 78-83-1, reactions 92-66-0, 4-Bromobiphenyl 97-99-4,

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Tetrahydrofurfuryl alcohol 99-90-1, 4'-Bromoacetophenone
                                                         106-52-5,
4-Hydroxy-1-methylpiperidine 107-21-1, Ethylene glycol, reactions
107-30-2, Chloromethyl methyl ether 108-01-0, 2-
Dimethylaminoethanol 127-08-2 141-53-7, Sodium formate
516-12-1, N-Iodosuccinimide 578-57-4, 2-Bromoanisole 583-70-0,
4-Bromo-m-xylene 593-71-5, Chloroiodomethane 619-42-1, Methyl
4-bromobenzoate 622-40-2, N-(2-Hydroxyethyl)morpholine 626-60-8,
3-Chloropyridine 688-73-3, Tributyltin hydride 865-47-4 1333-83-1,
Sodium hydrogen fluoride 1589-49-7, 3-Methoxy-1-propanol 1817-88-5,
2-(Cyclohexyloxy)ethanol 2051-62-9, 4-Chlorobiphenyl 2052-49-5,
Tetrabutylammonium hydroxide 2081-44-9 2398-37-0, 3-Bromoanisole
2516-33-8, Cyclopropylmethanol 2842-38-8, N-Cyclohexylethanolamine
2919-23-5, Cyclobutanol 3040-44-6, 1-Piperidineethanol 3188-13-4,
Ethoxymethyl chloride 3400-45-1, Cyclopentanecarboxylic acid
3970-21-6, 2-Methoxyethoxymethyl chloride 4441-30-9,
N-(3-Hydroxypropyl)morpholine 5332-24-1, 3-Bromoquinoline
                                                          5419-55-6,
Triisopropylborate 5464-12-0, 1-(2-Hydroxyethyl)-4-methylpiperazine
7789-29-9, Potassium hydrogen fluoride 13195-50-1,
2-Bromo-5-nitrothiophene 13330-96-6, 4-(Dimethylamino)-1-butanol
17763-80-3, 4-Nitrophenyl trifluoromethanesulfonate 30525-89-4,
Paraformaldehyde 41492-05-1, 1-Bromo-4-butylbenzene 109431-87-0
910251-09-1
RL: RCT (Reactant); RACT (Reactant or reagent)
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(preparation of hydroxymethylboron derivs. for hydroxymethylation or alkoxymethylation of aromatic rings)

IT 910251-10-4P 910251-11-5P 910251-13-7P 910251-14-8P 910251-15-9P
910251-18-2P 910251-28-4P 910251-34-2P 910251-35-3P 910251-38-6P
RL: RCT (Reactant); RGT (Reagent); SPN (Synthetic preparation); PREP
(Preparation); RACT (Reactant or reagent)

(preparation of hydroxymethylboron derivs. for hydroxymethylation or alkoxymethylation of aromatic rings)

IT 1067-44-3P 2842-41-3P 27490-32-0P 27490-33-1P 66222-29-5P,
Tributyliodomethyltin 83622-42-8P 166330-03-6P 201475-11-8P 393863-16-6P 393863-17-7P 910251-47-7P 910251-48-8P 910251-49-9P 910251-50-2P 910251-51-3P 910251-52-4P 910251-53-5P 910251-54-6P 910251-55-7P 910251-56-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of hydroxymethylboron derivs. for hydroxymethylation or alkoxymethylation of aromatic rings)

IIT 910251-12-6P 910251-16-0P 910251-17-1P 910251-19-3P 910251-20-6P
910251-22-8P 910251-23-9P 910251-24-0P 910251-25-1P 910251-26-2P
910251-27-3P 910251-29-5P 910251-30-8P 910251-31-9P 910251-32-0P
910251-33-1P 910251-36-4P 910251-37-5P
RL: RGT (Reagent); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of hydroxymethylboron derivs. for hydroxymethylation or alkoxymethylation of aromatic rings)

II 100-55-0P, 3-Pyridinemethanol 1515-83-9P 1719-82-0P 3597-91-9P, [1,1'-Biphenyl]-4-methanol 21998-86-7P 22072-50-0P 72390-19-3P, 858842-81-2P 910251-33-7P 910251-40-0P 910251-41-1P 910251-42-2P 910251-43-3P 910251-44-4

(preparation of hydroxymethylboron derivs. for hydroxymethylation or alkoxymethylation of aromatic rings)

RE.CNT 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD

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- L9 ANSWER 11 OF 55 CAPLUS COPYRIGHT 2009 ACS on STN
- AN 2006:920607 CAPLUS
- DN 145:326331
- ED Entered STN: 08 Sep 2006
- TI Method to remove resist, etch residue, and copper oxide from substrates having copper and low-k dielectric material
- IN Suzuki, Tomoko; Hiraga, Toshitaka; Katsuya, Yasuo; Reid, Chris
- PA Ekc Technology, Inc., USA
- SO PCT Int. Appl., 54pp.
 - CODEN: PIXXD2
 T Patent
- DT Patent LA English
- CC 76-3 (Electric Phenomena)
 - Section cross-reference(s): 48

FAN.CNT 1

PATENT NO.						KIND DATE					APPLICATION NO.								
PI	WO	2006	O937 AE, CN, GE, KZ, MZ, SG, VN,	70 AG, CO, GH, LC, NA, SK, YU,	AL, CR, GM, LK, NG, SL, ZA,	A1 AM, CU, HR, LR, NI, SM, ZM,	AT, CZ, HU, LS, NO, SY,	2006 AU, DE, ID, LT, NZ, TJ,	DK, DK, IL, LU, OM, TM,	BA, DM, IN, LV, PG, TN,	WO 2 BB, DZ, IS, LY, PH, TR,	BG, EC, JP, MA, PL, TT,	US63 BR, EE, KE, MD, PT, TZ,	78 BW, EG, KG, MG, RO, UA,	BY, ES, KM, MK, RU, UG,	BZ, FI, KN, MN, SC, US,	GB, KP, MW, SD, UZ,	CH, GD, KR, MX, SE, VC,	
			IS, CF, GM,	IT, CG, KE,	LT, CI, LS,	LU, CM, MW, RU,	LV, GA, MZ,	MC, GN, NA,	NL, GQ,	PL, GW, SL,	PT, ML, SZ,	RO, MR, TZ,	SE, NE, UG,	SI, SN, ZM,	SK, TD,	TR,	BF, BW,	BJ, GH,	
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		0937		IPC	I	G03F	0007 *]	-42	[I,A]; H	01L0	021-	3213	[I,	A];	H01L	0021		
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US				IPC NCL ECL	I A	H01L021/311C2; H01L021/3213C2 C11D0007-32 [I,A]; C11D0007-22 [I,C*] 510/175.000 C11D007/10; C11D007/26C; C11D007/26E; C11D007/32B; C11D007/32E; C11D007/36; C11D011/00BZD8													
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JP	JP 2008532289			IPC	Ι	H01L021/311C2; H01L021/3213C2 H01L0021-304 [I,A]; C11D0007-26 [I,A]; C11D0007-50 [I,A]; C11D0007-32 [I,A]; C11D0007-10 [I,A];										50			

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[I,A]; C11D0007-22 [I,C*]; H01L0021-3213 [I,A];
                       H01L0021-3205 [I,A]; H01L0021-02 [I,C*]; H01L0023-52
                       [I.A]
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                       5F033/QQ93; 5F033/QQ94; 5F033/RR04; 5F033/SS04;
                       5F033/WW00; 5F033/WW03; 5F033/WW04; 5F033/XX01;
                       5F033/XX21; 5F157/AA32; 5F157/AA35; 5F157/AA63;
                       5F157/AA64; 5F157/AA69; 5F157/AA70; 5F157/AA93;
                       5F157/AA96; 5F157/AB02; 5F157/AB03; 5F157/AB89;
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                       5F157/BD03; 5F157/BD52; 5F157/BE12; 5F157/BE42;
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JP 2008277718 IPCI
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                       C11D0007-02 [I,C*]; C11D0007-36 [I,A]; C11D0007-22
                       [I,C*]; C11D0007-50 [I,A]; H01L0021-027 [I,A];
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                       5F157/CB02; 5F157/CB03; 5F157/CB23; 5F157/DB18
KR 2007106038 IPCI
                      H01L0021-304 [I,A]; H01L0021-02 [I,C*]
CN 101228481
                IPCI
                      G03F0007-42 [I,A]; H01L0021-3213 [I,A]; H01L0021-02
                       [I,C*]
    A variety of compns, that are particularly applicable for removing one or
    more of resist, etching residue, planarization residue, and Cu oxide from
    a substrate comprising Cu and a low-k dielec, material are described. The
    resist, residues, and Cu oxide are removed by contacting the substrate
    surface with the composition, typically for a period of 30 s to 30 min, and at
    a temperature between 25 and 45°. The composition includes a
    fluoride-providing component; at least 1% by weight of a H2O miscible organic
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C11D0007-08 [I,A]; C11D0007-02 [I,C*]; C11D0007-36

- further includes up to about 0.4% of one or more chelators.
- ST resist cleaning etch residue copper oxide low const dielec
- IT Polishing

composition

(Chemical-mech., residues from; method and compns. to remove resist, etch residue, and copper oxide from substrates having copper and low-constant dielec. material)

IT Dielectric films

(low- κ ; method and compns. to remove resist, etch residue, and copper oxide from substrates having copper and low-constant dielec.material)

solvent; an organic acid; and at least 81% by weight H2O. Typically the

IT Cleaning

Photoresists

(method and compns. to remove resist, etch residue, and copper oxide

from substrates having copper and low-constant dielec. material)

IT Etching

(residues from; method and compns. to remove resist, etch residue, and copper oxide from substrates having copper and low-constant dielec. material)

IT Chelating agents

(solns. containing; method and compns. to remove resist, etch residue, and copper oxide from substrates having copper and low-constant dielec. material)

IT 60-00-4, Ethylenediaminetetraacetic acid, processes 67-43-6, Diethylenetriaminepentaacetic acid

RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); TEM (Technical or engineered material use); PROC (Process); USES (USes)

(chelator; method and compns. to remove resist, etch residue, and copper oxide from substrates having copper and low-constant dielec. material)

IT 52-90-4, L-Cysteine, processes 56-40-6, Glycine, processes 56-41-7,
L-Alanine, processes 77-92-9, Citric acid, processes 100-37-8,
2-Diethylaminoethanol 108-01-0, Dimethylaminoethanol
111-77-3, Diethylene glycol monomethyl ether 112-34-5, Diethylene glycol

monobutyl ether 1320-67-8, Propylene glycol monomethyl ether 2809-21-4 4746-62-7, Hydroxyglycine 7664-39-3, Hydrogen fluoride, processes 10043-35-3, Boric acid, processes 12125-01-8, Ammonium fluoride 13598-36-2, Phosphonic acid 52125-53-8, Propylene glycol monoethyl ether

RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); TEM (Technical or engineered material use); PROC (Process); USES (Uses)

(cleaning composition; method and compns. to remove resist, etch residue, and copper oxide from substrates having copper and low-constant dielec. material)

IT 50-81-7, Ascorbic acid, uses 64-18-6, Formic acid, uses 79-14-1, Glycolic acid, uses 87-69-4, Tartaric acid, uses 144-62-7, Oxalic acid, uses 563-96-2, Glyoxylic acid monohydrate RL: NUU (Other use, unclassified); USES (Uses)

(cleaning composition; method and compns. to remove resist, etch residue, and copper oxide from substrates having copper and low-constant dielec. material)

IT 1344-70-3, Copper oxide

RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); REM (Removal or disposal); PROC (Process)

(method and compns. to remove resist, etch residue, and copper oxide from substrates having copper and low-constant dielec. material)

IT 7440-50-8, Copper, uses

RL: DEV (Device component use); USES (Uses)

(method and compns. to remove resist, etch residue, and copper oxide from substrates having copper and low-constant dielec. material)

RE.CNT 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD

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- (2) Kanto Kagaku Kabushiki Kaisha; EP 1347339 A 2003 CAPLUS
- (3) Kanto Kagaku Kabushiki Kaisha; EP 1612611 A 2006 CAPLUS
- (4) Lee, S; US 2004038840 Al 2004 CAPLUS
- L9 ANSWER 12 OF 55 CAPLUS COPYRIGHT 2009 ACS on STN
- AN 2006:655920 CAPLUS
- DN 145:124613
- ED Entered STN: 07 Jul 2006
 - I Preparation of carboxylic acid derivatives having three cyclic moieties as anticoagulants
- IN Ishihara, Tsukasa; Miura, Masanori; Ohne, Kazuhiko; Takuwa, Tomofumi; Shirakami, Shohei; Ibuka, Ryotaro; Ohnuki, Kei; Seki, Norio; Shigenaga,

Takeshi; Hirayama, Fukushi; Hirabayashi, Akihito; Kai, Yuichiro; Kobayashi, Junichi; Hirasawa, Hideaki; Kondou, Atsushi; Yamada, Ken

PA Astellas Pharma Inc., Japan

SO PCT Int. Appl., 198 pp.

CODEN: PIXXD2

DT Pat.ent.

LA Japanese

28-17 (Heterocyclic Compounds (More Than One Hetero Atom))

Section cross-reference(s): 1, 25, 27

FAN.CNT 1																		
PATENT NO.					KIND DATE			APPLICATION NO.				DATE						
PI	WO 2006070878			A1 2006		2006	060706			WO 2005-JP24096				20051228				
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			CN,	co,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	EG,	ES,	FI,	GB,	GD,
			GE,	GH,	GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	KE,	KG,	KM,	KN,	KP,	KR,
			ΚZ,	LC,	LK,	LR,	LS,	LT,	LU,	LV,	LY,	MA,	MD,	MG,	MK,	MN,	MW,	MX,
			MZ,	NA,	NG,	NI,	NO,	NZ,	OM,	PG,	PH,	PL,	PT,	RO,	RU,	SC,	SD,	SE,
			SG,	SK,	SL,	SM,	SY,	TJ,	TM,	TN,	TR,	TT,	TZ,	UA,	UG,	US,	UZ,	VC,
			VN,	YU,	ZA,	ZM,	ZW											
		RW:	ΑT,	BE,	BG,	CH,	CY,	CZ,	DE,	DK,	EE,	ES,	FI,	FR,	GB,	GR,	HU,	ΙE,
			IS,	IT,	LT,	LU,	LV,	MC,	NL,	PL,	PT,	RO,	SE,	SI,	SK,	TR,	BF,	ВJ,
			CF,	CG,	CI,	CM,	GA,	GN,	GQ,	GW,	ML,	MR,	NE,	SN,	TD,	TG,	BW,	GH,
			GM,	KE,	LS,	MW,	ΜZ,	NA,	SD,	SL,	SZ,	TZ,	UG,	ZM,	ZW,	AM,	ΑZ,	BY,
			KG,	KZ,	MD,	RU,	TJ,	TM										
DDAT	.TD	2004	-38n	131		Α		2004	1228									

CLASS

PATENT NO. CLASS PATENT FAMILY CLASSIFICATION CODES

_____ WO 2006070878 IPCI C07C0237-40 [I,A]; C07C0237-00 [I,C*]; C07C0255-13 [I,A]; C07C0255-00 [I,C*]; C07C0257-18 [I,A]; C07C0257-20 [I,A]; C07C0257-00 [I,C*]; C07C0259-18 [I,A]; C07C0259-00 [I,C*]; C07C0271-64 [I,A]; C07C0271-00 [I,C*]; C07C0307-06 [I,A]; C07C0307-10 [I,A]; C07C0307-00 [I,C*]; C07D0207-08 [I,A]; C07D0207-12 [I,A]; C07D0207-267 [I,A]; C07D0207-34 [I,A]; C07D0207-00 [I,C*]; C07D0209-14 [I,A]; C07D0209-42 [I,A]; C07D0209-00 [I,C*]; C07D0211-26 [I,A]; C07D0211-00 [I,C*]; C07D0213-30 [I,A]; C07D0213-75 [I,A]; C07D0213-81 [I,A]; C07D0213-82 [I,A]; C07D0213-84 [I,A]; C07D0213-00 [I,C*]; C07D0217-18 [I,A]; C07D0217-00 [I,C*]; C07D0231-12 [I,A]; C07D0231-00 [I,C*]; C07D0235-30 [I,A]; C07D0235-00 [I,C*]; C07D0237-24 [I,A]; C07D0237-00 [I,C*]; C07D0239-28 [I,A]; C07D0239-00 [I,C*]; C07D0241-04 [I,A]; C07D0241-08 [I,A]; C07D0241-26 [I,A]; C07D0241-00 [I,C*]; C07D0243-08 [I,A]; C07D0243-00 [I,C*]; C07D0263-32 [I,A]; C07D0263-00 [I,C*]; C07D0265-30 [I,A]; C07D0265-00 [I,C*]; C07D0271-06 [I,A]; C07D0271-10 [I,A]; C07D0271-00 [I,C*]; C07D0295-08 [I,A]; C07D0295-12 [I,A]; C07D0295-18 [I,A]; C07D0295-00 [I,C*]; C07D0307-52 [I,A]; C07D0307-00 [I,C*]; C07D0333-38 [I,A]; C07D0333-00 [I,C*]; C07D0401-04 [I,A]; C07D0401-00 [I,C*]; A61K0031-195 [I,A]; A61K0031-185 [I,C*]; A61K0031-216 [I,A]; A61K0031-27 [I,A]; A61K0031-21 [I,C*]; A61K0031-277 [I,A]; A61K0031-275 [I,C*]; A61K0031-337 [I,A]; A61K0031-40 [I,A]; A61K0031-4015 [I,A]; A61K0031-4045 [I,A]; A61K0031-415 [I,A]; A61K0031-4184 [I,A]; A61K0031-4164 [I,C*]; A61K0031-44 [I,A]; A61K0031-445 [I,A]; A61K0031-495 [I,A]; A61K0031-4965 [I,A]; A61K0031-5375 [I,A]; A61K0031-4409

[I,A]; A61K0031-4418 [I,A]; A61K0031-455 [I,A]; A61K0031-551 [I,A]; A61K0031-341 [I,A]; A61K0031-421 [I,A]; A61K0031-472 [I,A]; A61K0031-404 [I,A]; A61K0031-403 [I,C*]; A61K0031-4245 [I,A]; A61K0031-50 [I,A]; A61K0031-505 [I,A]; A61K0031-4439 [I,A]; A61K0031-4427 [I,C*]; A61K0031-381 [I,A]; A61P0007-02 [I,A]; A61P0007-00 [I,C*]; A61P0009-10 [I,A]; A61P0009-00 [I,C*]; A61P0043-00 [I,A] IPCR C07C0237-00 [I,C]; C07C0237-40 [I,A]; A61K0031-185 [I,C]; A61K0031-195 [I,A]; A61K0031-21 [I,C]; A61K0031-216 [I,A]; A61K0031-27 [I,A]; A61K0031-275 [I,C]; A61K0031-277 [I,A]; A61K0031-337 [I,C]; A61K0031-337 [I,A]; A61K0031-341 [I,C]; A61K0031-341 [I,A]; A61K0031-381 [I,C]; A61K0031-381 [I,A]; A61K0031-40 [I,C]; A61K0031-40 [I,A]; A61K0031-4015 [I,C]; A61K0031-4015 [I,A]; A61K0031-403 [I,C]; A61K0031-404 [I,A]; A61K0031-4045 [I,A]; A61K0031-415 [I,C]; A61K0031-415 [I,A]; A61K0031-4164 [I,C]; A61K0031-4184 [I,A]; A61K0031-421 [I,C]; A61K0031-421 [I,A]; A61K0031-4245 [I,C]; A61K0031-4245 [I,A]; A61K0031-44 [I,C]; A61K0031-44 [I,A]; A61K0031-4409 [I,C]; A61K0031-4409 [I,A]; A61K0031-4418 [I,C]; A61K0031-4418 [I,A]; A61K0031-4427 [I,C]; A61K0031-4439 [I,A]; A61K0031-445 [I,C]; A61K0031-445 [I,A]; A61K0031-455 [I,C]; A61K0031-455 [I,A]; A61K0031-472 [I,C]; A61K0031-472 [I,A]; A61K0031-495 [I,C]; A61K0031-495 [I,A]; A61K0031-4965 [I,C]; A61K0031-4965 [I,A]; A61K0031-50 [I,C]; A61K0031-50 [I,A]; A61K0031-505 [I,C]; A61K0031-505 [I,A]; A61K0031-5375 [I,C]; A61K0031-5375 [I,A]; A61K0031-551 [I,C]; A61K0031-551 [I,A]; A61P0007-00 [I,C]; A61P0007-02 [I,A]; A61P0009-00 [I,C]; A61P0009-10 [I,A]; A61P0043-00 [I,C]; A61P0043-00 [I,A]; C07C0255-00 [I,C]; C07C0255-13 [I,A]; C07C0257-00 [I,C]; C07C0257-18 [I,A]; C07C0257-20 [I,A]; C07C0259-00 [I,C]; C07C0259-18 [I,A]; C07C0271-00 [I,C]; C07C0271-64 [I,A]; C07C0307-00 [I,C]; C07C0307-06 [I,A]; C07C0307-10 [I,A]; C07D0207-00 [I,C]; C07D0207-08 [I,A]; C07D0207-12 [I,A]; C07D0207-267 [I,A]; C07D0207-34 [I,A]; C07D0209-00 [I,C]; C07D0209-14 [I,A]; C07D0209-42 [I,A]; C07D0211-00 [I,C]; C07D0211-26 [I,A]; C07D0213-00 [I,C]; C07D0213-30 [I,A]; C07D0213-75 [I,A]; C07D0213-81 [I,A]; C07D0213-82 [I,A]; C07D0213-84 [I,A]; C07D0217-00 [I,C]; C07D0217-18 [I,A]; C07D0231-00 [I,C]; C07D0231-12 [I,A]; C07D0235-00 [I,C]; C07D0235-30 [I,A]; C07D0237-00 [I,C]; C07D0237-24 [I,A]; C07D0239-00 [I,C]; C07D0239-28 [I,A]; C07D0241-00 [I,C]; C07D0241-04 [I,A]; C07D0241-08 [I,A]; C07D0241-26 [I,A]; C07D0243-00 [I,C]; C07D0243-08 [I,A]; C07D0263-00 [I,C]; C07D0263-32 [I,A]; C07D0265-00 [I,C]; C07D0265-30 [I,A]; C07D0271-00 [I,C]; C07D0271-06 [I,A]; C07D0271-10 [I,A]; C07D0295-00 [I,C]; C07D0295-08 [I,A]; C07D0295-12 [I,A]; C07D0295-18 [I,A]; C07D0307-00 [I,C]; C07D0307-52 [I,A]; C07D0333-00 [I,C]; C07D0333-38 [I,A]; C07D0401-00 [I,C]; C07D0401-04 [I,A] ECLA C07D211/32; C07C237/40; C07C255/13; C07C257/18; C07C257/20; C07C259/18; C07C271/64; C07C307/06; C07C307/10; C07C311/08; C07C311/37; C07C317/32; C07C323/32; C07C323/52; C07D207/08; C07D207/12;

C07D207/267; C07D207/34; C07D209/14; C07D209/42;

COTD211/26; COTD213/30; COTD213/75; COTD213/81; COTD213/82; COTD213/84; COTD213/84; COTD213/82; COTD231/12; COTD235/30; COTD237/24; COTD239/28; COTD241/04; COTD241/08; COTD241/26; COTD243/08; COTD263/32; COTD263/30; COTD271/26; COTD2671/10; COTD265/38; COTD265/30; COTD271/10; COTD271/10; COTD265/08; COTD295/18; COTD301/04; MOTD; MOTD;

OS MARPAT 145:124613 GI

$$(R^4)_{p} \xrightarrow{C} X - Y \xrightarrow{\bigcap} R^5$$

$$(R^2)_{m} \xrightarrow{A} J \xrightarrow{B} (R^3)_{n}$$

The title compds. [I; ring A = aryl or heteroaryl ring; ring B = benzene, AB naphthalene, or monocyclic or bicyclic heteroaryl ring; ring C = cycloalkyl, aryl, or heterocyclic ring; m, n, p = an integer of 0-3; R1 = NH2, CH2NH2, CONH2, C(:NH)NH2, C(:NOH)NH2, C(:NH)NH-CO2-(optionally substituted lower alkyl), 5-oxo-2,5-dihydro-1,2,4-oxadiazol-3-yl; R2, R3 = lower alkyl, halo-lower alkyl, halo, oxo, cyano, NO2, halo-lower alkoxy, NROROO, SRO, S(O)RO, SO2RO, SO2NROROO, NROSO2ROO, CORO, CO2RO, CONROROO, NROCOROO, NROCO-(halo-lower alkyl), cycloalkyl, aryl, heterocyclyl, etc.; RO, ROO = H, lower alkyl; R4 = lower alkyl, lower alkenyl, cycloalkyl, aryl, heterocyclyl, halo, oxo, cyano, NO2, OR6, NR6R6a, SR6, SOR6, SO2R6, SOZNR6R6a, NR6SOZR6a, NR6SOZNR6R6a, NR6SOZNR6aCOZR6a, COR6, COZR6, CONR6R6a, cycloalkyl, aryl, heterocyclyl, etc.; R6, R6a = H, each (un) substituted lower alkyl, lower alkenyl, cycloalkyl, aryl, or heterocyclyl; R5 = ORO, NROROO, N(RO)-lower alkylene-OROO; J = NROCO, CONRO, NROCONRO, NRO-lower alkylene, lower alkylene-NROCO; L = NRO-lower alkylene, NRO-lower alkenylene, lower alkylene, lower alkenylene; X = a single bond, (un)substituted NH, S, CO, SO, SO2, lower alkylene-O, lower alkylene-(un)substituted NH; Y = a single bond, each (un)substituted lower alkylene or lower alkenylene] or pharmaceutically acceptable salt thereof are prepared These compds. such as phenoxyacetic acid and phenylpropanoic acid derivs. or salts thereof have an anticoagulant effect based on the inhibition of the activated blood coagulation factor VII and, therefore, are useful as blood coagulation inhibitors or preventives/remedies for diseases caused by thrombus or embolus. They are also selective inhibitors of activated blood coagulation factor VII over activated blood coagulation factor X and thrombin. The above diseases include ischemic heart diseases, restenosis after angioplasty, cerebral thrombosis, transient cerebral ischemia, peripheral arterial obstruction, Charcot's syndrome (intermittent claudication), deep venous thrombosis, pulmonary embolism, disseminated intravascular coagulation (DIC), thrombogenesis after heart valve replacement surgery, coagulation or inflammation of circulating blood during external blood circulation, arteriosclerosis, and cancer. For example, [(3-([(2-([(2-amino-1H-benzimidazol-5y1)amino]carbony1)-4-chloropheny1)amino]methy1)bipheny1-2-y1)oxy]acetic acid in vitro inhibited activated blood coagulation factor VII over activated blood coagulation factor X and thrombin with IC50 of 0.36, ≥ 100 , and ≥ 100 μM , resp.

phenylpropanoic acid prepn anticoagulant; phenoxyacetic acid prepn

anticoagulant; activated blood coagulation factor VII inhibitor phenoxyacetic acid prepn; carboxylic acid contg cyclic group prepn anticoagulant; thrombus embolus treatment prevention phenoxyacetic acid phenyloropanoic acid prepn

Ischemia

(cardiac; preparation of carboxylic acid derivs. having three cyclic moieties as activated blood coagulation factor VII inhibitors and anticoagulants)

IT Blood coagulation

(coagulation of circulating blood during external blood circulation; preparation of carboxylic acid derivs. having three cyclic moieties as activated blood coagulation factor VII inhibitors and anticoagulants)

IT Artery, disease

(coronary, restenosis, after angioplasty; preparation of carboxylic acid derivs. having three cyclic moleties as activated blood coagulation factor VII inhibitors and anticoagulants)

IT Blood coagulation disorders

Blood coagulation disorders

(disseminated intravascular coagulation; preparation of carboxylic acid derivs. having three cyclic moleties as activated blood coagulation factor VII inhibitors and anticoaculants)

IT Lung, disease

(embolism; preparation of carboxylic acid derivs. having three cyclic moieties as activated blood coagulation factor VII inhibitors and anticoagulants)

IT Anti-inflammatory agents

Inflammation

(inflammation of circulating blood during external blood circulation; preparation of carboxylic acid derivs. having three cyclic moieties as activated blood coagulation factor VII inhibitors and anticoagulants)

IT Artery, disease

(intermittent claudication, Charcot's syndrome; preparation of carboxylic acid derivs. having three cyclic moieties as activated blood coaqulation factor VII inhibitors and anticoaqulants)

IT Brain, disease

(ischemia, transient; preparation of carboxylic acid derivs. having three cyclic moieties as activated blood coagulation factor VII inhibitors and anticoagulants)

IT Heart, disease

(ischemia; preparation of carboxylic acid derivs. having three cyclic moieties as activated blood coagulation factor VII inhibitors and anticoagulants)

Artery, disease

(occlusion, peripheral; preparation of carboxylic acid derivs. having three cyclic moieties as activated blood coagulation factor VII inhibitors and anticoagulants)

Antiarteriosclerotics

Anticoagulants
Antitumor agents
Arteriosclerosis
Embolism
Neoplasm

Thrombosis

(preparation of carboxylic acid derivs. having three cyclic moieties as activated blood coagulation factor VII inhibitors and anticoagulants)

IT Carboxylic acids, preparation Fatty acids, preparation

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of carboxylic acid derivs. having three cyclic moieties as activated blood coagulation factor VII inhibitors and anticoagulants) $\,$

IT Embolism

(pulmonary; preparation of carboxylic acid derivs. having three cyclic moleties as activated blood coagulation factor VII inhibitors and anticoagulants)

IT Brain, disease

(stroke; preparation of carboxylic acid derivs. having three cyclic moieties as activated blood coagulation factor VII inhibitors and anticoagulants)

IT Thrombus

(thrombogenesis after heart valve replacement surgery; preparation of carboxylic acid derivs. having three cyclic moieties as activated blood coagulation factor VII inhibitors and anticoagulants)

IT Ischemia

(transient cerebral; preparation of carboxylic acid derivs. having three cyclic moieties as activated blood coagulation factor VII inhibitors and anticoagulants)

IT Thrombosis

(venous; preparation of carboxylic acid derivs. having three cyclic moieties as activated blood coagulation factor VII inhibitors and anticoagulants)

IT 65312-43-6, Activated blood coagulation factor VII
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(inhibitors; preparation of carboxylic acid derivs. having three cyclic
moleties as activated blood coagulation factor VII inhibitors and
anticoagulants)

2357-33-7P, 4-Fluoro-2-(hydroxymethyl)phenol 2973-71-9P, 3-Ethoxy-5-formyl-4-hydroxybenzyl chloride 147291-56-3P, tert-Butyl [(4-aminophenyl)(imino)methyl]carbamate 183380-81-6P, Ethyl 2-(4-hydroxy-3-nitrophenyl)acetate 286437-63-6P, tert-Butyl 2-(2-formylphenoxy)acetate 400648-67-1P, Ethyl 2-[3-nitro-4-[[(trifluoromethyl)sulfonyl]oxy]phenyl]acetate 773094-22-7P, 2-(3-Methoxy-2-nitrophenyl)dioxolane 805952-10-7P, 4-[(Dimethylamino)methyl]-2-ethoxy-6-formylphenol 861442-04-8P, 4-Chloro-2-(hydroxymethyl)-6-iodophenol 897639-34-8P, [4-(Acetoxymethy1)-2-[[[3-[[[4-[amino(imino)methyl]phenyl]amino]carbonyl]pyridin-2-yl]amino]methyl]-6ethoxyphenoxy]acetic acid trifluoroacetate 897641-74-6P, tert-Butyl 2-[2-(2-hydroxyethyl)piperidin-1-yl]acetate 897641-75-7P, tert-Butyl 3-[2-(hydroxymethyl)piperidin-1-yl]propanoate 897641-76-8P, tert-Butyl 3-(2-formylpiperidin-1-v1)propanoate 897641-77-9P, 5-Cvano-3-methoxysalicylaldehyde 897641-78-0P, 6-Chloro-8-iodo-2-phenvl-4H-1,3-benzodioxin 897641-79-1P. 1-[5-Chloro-2-hydroxy-3-(hydroxymethyl)phenyl]-4-methylpiperazin-2-one 897641-80-4P, 3-Ethoxy-5-formyl-4-hydroxybenzyl acetate 5-[(Dimethylamino)methyl]-2-hydroxy-3-isopropoxybenzaldehyde 897641-82-6P, 3-Formyl-4-hydroxy-5-isopropoxybenzyl acetate 897641-83-7P, 3,4-Dihydroxy-5-formylbenzyl acetate 897641-84-8P, 2-Hydroxy-5-iodo-3-isopropoxybenzaldehyde 897641-85-9P, 5-Formyl-2-hydroxy-3-isopropoxybenzyl acetate 897641-86-0P, tert-Butvl 2-[2-ethoxy-4-(2-hydroxyethy1)-6-(hydroxymethy1)phenoxy]acetate 897641-87-1P, tert-Butyl 2-(2-formyl-6-isopropoxy-4-vinylphenoxy)acetate 897641-88-2P, tert-Butyl 2-[4-(2-hydroxyethyl)-2-(hydroxymethyl)-6-897641-89-3P, Ethyl isopropoxyphenoxylacetate 2-[4-((1S)-1,2-dihydroxyethyl)-2-formyl-6-isopropoxyphenoxy]acetate 897641-90-6P, tert-Butyl 2-[2-ethoxy-6-formyl-4-[(2hydroxyethyl) (methyl) amino] phenoxy] acetate 897641-91-7P, tert-Butyl 2-[4-acetoxymethyl-2-(2-tert-butoxy-1-methylethoxy)-6formylphenoxylacetate 897641-92-8P, Ethyl 2-(2-acetoxymethyl-4-hydroxy-6-isopropoxyphenoxy)acetate 897641-93-9P, Ethyl 2-[4-[(tert-butyldimethylsilyl)oxy]-2-hydroxymethyl-6isopropoxyphenoxy]acetate 897641-94-0P 897641-95-1P, tert-Butyl (E)-3-(4-acetoxymethy1-2-formy1-6-isopropoxypheny1)-2-propenoate

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897641-96-2P, 2-Bromo-3-isopropoxy-5-nitrobenzaldehyde 897641-97-3P,
tert-Butyl (E)-3-(2-formyl-6-isopropoxy-4-nitrophenyl)-2-propenoate
897641-98-4P, tert-Butyl 3-(4-acetoxymethyl-2-hydroxymethyl-6-
isopropoxyphenyl)propanoate 897641-99-5P, tert-Butyl
3-[4-[[2-[(tert-butyldimethylsily1)oxy]ethyl]amino]-2-hydroxymethyl-6-
isopropoxyphenyl]propanoate 897642-00-1P, tert-Butyl
3-[4-[(tert-butoxycarbonyl)[2-[(tert-butyldimethylsilyl)oxy]ethyl]amino]-2-
hydroxymethyl-6-isopropoxyphenyl]propanoate 897642-01-2P, tert-Butyl
3-[4-[(tert-butoxycarbonv1)[2-[(tert-butvldimethylsilv1)oxy]ethyl]amino]-2-
formyl-6-isopropoxyphenyllpropanoate 897642-02-3P, Ethyl
3-[2-formyl-4-(2-hydroxyethylamino)-6-isopropoxyphenyl]propanoate
897642-03-4P, tert-Butyl 2-(4-acetoxymethyl-2-formyl-6-
isopropoxyphenyl)acetate 897642-04-5P, Ethyl
2-(2-formyl-4-hydroxymethyl-6-isopropoxyphenyl)acetate 897642-05-6P,
3-(2-Ethoxy-6-formylphenoxy)propanoic acid 897642-06-7P, tert-Butyl
2-[(3-formylbiphenyl-2-yl)oxy]acetate 897642-07-8P, tert-Butyl
2-[[[2-(hydroxymethyl)phenyl]methyl](methyl)amino]acetate 897642-08-9P,
tert-Butyl 2-[(tert-butoxycarbonyl)][2-
                                           897642-09-0P, tert-Butyl
(hydroxymethyl)phenyl]methyl]amino]acetate
2-[2-(dimethylamino)-6-(hydroxymethyl)phenoxy]acetate 897642-10-3P,
tert-Butyl 2-[2-formyl-4-(2-hydroxyethyl)-6-isopropoxyphenoxylacetate
897642-11-4P, tert-Butyl 2-[2-(1,3-dioxolan-2-yl)-6-
(methylsulfanyl)phenoxylacetate 897642-12-5P, tert-Butyl
2-[2-(1,3-dioxolan-2-v1)-6-(methylsulfonyl)phenoxylacetate
                                                           897642-13-6P.
[2-Formy1-6-(methylsulfanyl)phenoxy]acetic acid 897642-14-7P, tert-Butyl
2-[2-[2-(dimethylamino)propoxy]-6-formylphenoxy]acetate
                                                       897642-15-8P.
tert-Butyl 2-[4-amino-2-(hydroxymethyl)-6-methoxyphenoxy]acetate
897642-16-9P, tert-Butyl 2-[2-(hydroxymethyl)-6-methoxy-4-
(methylamino)phenoxy]acetate
                             897642-17-0P, tert-Butyl
2-[4-[(tert-butoxycarbonyl)(methyl)amino]-2-formyl-6-
methoxyphenoxy]acetate 897642-18-1P, tert-Butyl
2-[4-(dimethylamino)-2-formyl-6-methoxyphenoxy]acetate 897642-19-2P,
tert-Buty1 2-[4-(acetylamino)-2-formy1-6-methoxyphenoxy]acetate
897642-20-5P, tert-Butyl 2-[4-[(dimethylamino)methyl]-2-ethoxy-6-
                      897642-21-6P, tert-Butyl
formvlphenoxvlacetate
2-[4-[[bis(tert-butoxycarbonyl)amino]methyl]-2-ethoxy-6-
formylphenoxy]acetate
                      897642-22-7P, tert-Butyl
3-(2-formylphenyl)propanoate 897642-23-8P, tert-Butyl
2-[(2-formyl-6-methoxyphenyl)(methyl)amino]acetate 897642-24-9P,
N-[2-(1,3-Dioxolan-2-v1)phenyl]-2,2,2-trifluoro-N-methylacetamide
             897642-26-1P, tert-Butvl
[[4-[(2-amino-5-chlorobenzyl)amino]phenyl](imino)methyl]carbamate
897642-27-2P, 2-[[2-(2-tert-Butoxy-2-oxoethoxy)benzyl]amino]-5-
chlorobenzoic acid
                   897642-28-3P, Ethyl
[(4-aminophenyl)(imino)methyl]carbamate
                                        897642-29-4P, Ethyl
2-(3-nitro-4-vinvlphenvl)acetate 897642-30-7P, Ethyl
                                 897642-31-8P,
2-(4-formvl-3-nitrophenvl)acetate
4-[(Ethoxycarbonvl)methyl]-2-nitrobenzoic acid 897642-32-9P, tert-Butyl
2-[2-[[[2-[[[4-[[(tert-butoxycarbonyl)amino]methyl]phenyl]amino]carbonyl]-
4-chlorophenyl]amino]methyl]-6-ethoxyphenoxy]acetate 897642-33-0P,
tert-Butyl [[4-[(5-chloro-2-
nitrobenzovl)amino[phenyl](imino)methyl]carbamate 897642-34-1P,
tert-Butv1 [[5-[(5-chloro-2-nitrobenzov1)amino]pyridin-2-
yl](imino)methyl]carbamate
                            897642-35-2P, tert-Butvl
[[4-[[4-(2-amino-2-oxoethv1)-2-
nitrobenzoyl]amino]phenyl](imino)methyl]carbamate
                                                  897642-36-3P.
N-[4-[(Amino)(hydroxyimino)methyl]phenyl]-5-chloro-2-nitrobenzamide
897642-38-5P
              897642-39-6P 897642-40-9P, Hexyl
[imino[4-[(5-methy1-2-nitrobenzoy1)amino]pheny1]methy1]carbamate
897642-41-0P, tert-Butyl 2-[2-ethoxy-6-
[(hydroxyimino)methyl]phenoxy]acetate 897642-42-1P, tert-Butyl
[[4-[(2-amino-5-chlorobenzoyl)amino]phenyl](imino)methyl]carbamate
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897642-43-2P, 2-Amino-N-[4-[(amino)(hydroxyimino)methyl]phenyl]-5-
                897642-44-3P, tert-Butvl
methylbenzamide
[[4-](2-amino-5-bromobenzov1)amino[pheny1](imino)methy1]carbamate
897642-45-4P, tert-Butv1 2-[2-[[(4-chloro-2-nitrophenv1)amino]methv1]-6-
ethoxyphenoxy]acetate 897642-46-5P, tert-Butyl
2-[2-[[[4-chloro-2-[(4-cyanobenzoy1)amino]phenyl]amino]methyl]-6-
ethoxyphenoxy]acetate 897642-47-6P, Ethyl
2-[2-formyl-4-(hydroxymethyl)-6-isopropoxyphenoxy]acetate 897642-48-7P,
2-Benzyloxy-3-(2-tert-butoxy-1-methylethoxy)benzaldehyde 897642-49-8P,
3-(2-tert-Butoxy-1-methylethoxy)-2-hydroxybenzaldehyde 897642-50-1P
897642-51-2P 897642-52-3P, tert-Butvl
(E)-3-[4-acetoxymethyl-2-(2-acetoxy-1-methylethoxy)-6-formylphenyl]-2-
propenoate 897643-90-2P, 1-(6-Chloro-2-phenyl-4H-1,3-benzodioxin-8-yl)-4-
methylpiperazin-2-one 897643-92-4P, Ethyl
2-(2-acetoxymethyl-4-formyloxy-6-isopropoxyphenoxy)acetate 897643-93-5P,
Ethyl 2-[4-[(tert-butyldimethylsilyl)oxy]-2-(acetoxymethyl)-6-
isopropoxyphenoxy]acetate 897643-95-7P,
(4-Acetoxymethyl-2-formyl-6-isopropoxyphenyl)acetic acid 897643-96-8P,
tert-Butyl 2-(2-formyl-6-hydroxyphenoxy)acetate 897643-97-9P, tert-Butyl
2-[2-formyl-6-[(trifluoromethylsulfonyl)oxy]phenoxy]acetate
897643-98-0P, tert-Butvl 2-|||2-
(acetoxymethyl)phenyl|methyl|(methyl)amino|acetate
tert-Butvl 2-[[[2-(acetoxymethyl)phenyl]methyl]amino]acetate
897644-00-7P, tert-Butvl 2-1(tert-butoxycarbonyl)[[2-
                                           897644-01-8P, tert-Butvl
(acetoxymethyl)phenyl]methyl]amino]acetate
                                              897644-02-9P, tert-Butyl
2-[4-fluoro-2-(hydroxymethyl)phenoxy]acetate
2-(4-fluoro-2-formylphenoxy)acetate 897644-03-0P, tert-Butyl
2-(2-ethoxy-6-formyl-4-hydroxymethylphenoxy)acetate 897644-04-1P,
2-[3-Methoxy-2-[(trifluoroacetyl)amino]phenyl]dioxolane
                                                        897644-05-2P.
2-[3-Methoxy-2-[N-(trifluoroacetyl)-N-methylamino]phenyl]dioxolane
897644-06-3P, 2-[3-Methoxy-2-(methylamino)phenyl]dioxolane
tert-Butyl 2-[[2-(dioxolan-2-yl)-6-methoxyphenyl](methyl)amino]acetate
897644-10-9P, N-[2-(Dioxolan-2-v1)phenv1]-2,2,2-trifluoroacetamide
897644-12-1P, N-[2-(Dioxolan-2-vl)phenvl]-N-methylamine
                                                        897644-13-2P,
tert-Butvl [[4-[(2-nitro-5-
chlorobenzyl)amino]phenyl](imino)methyl]carbamate
                                                  897644-15-4P.
[4-[[4-[[(tert-Butoxycarbonyl)amino](imino)methyl]phenyl]carbamoyl]-3-
nitrophenyl]acetic acid
                        897644-20-1P, tert-Butyl
2-[2-[1-[(4-chloro-2-hydroxymethylphenyl)amino]ethyl]phenoxy]acetate
897644-21-2P, tert-Butvl 2-[2-[1-[(4-chloro-2-
carboxyphenyl)aminolethyllphenoxylacetate 897644-22-3P, tert-Butyl
2-[2-[1-[[4-chloro-2-[[[4-[(tert-
butoxycarbonylamino)methyllphenyllamino|carbonyllphenyllamino|ethyllphenox
vlacetate
           897644-28-9P, tert-Butyl
[[4-[[2-[[[2-(ethoxycarbonylmethoxy)-3-isopropoxy-5-[(tert-
butyldimethylsilyl)oxylphenyl]methyl]amino]-5-
methylbenzoyl]amino]phenyl](imino)methyl]carbamate 897644-29-0P,
tert-Butyl [[4-[[2-[[[2-(ethoxycarbonylmethoxy)-3-isopropoxy-5-
hydroxyphenyllmethyllaminol-5-
methylbenzoyl]amino]phenyl](imino)methyl]carbamate 897644-30-3P,
tert-Butyl 2-[4-acetoxymethyl-2-[[[2-[[[4-[[(tert-
butoxycarbonyl)amino](imino)methyl]phenyl]amino]carbonyl]-4-
methylphenyl]amino]methyl]-6-(2-tert-butoxy-1-methylethoxy)phenoxylacetate
897644-35-8P, 3-[2-[[2-[2-(tert-Butoxycarbonyl)ethyl]-4-[[2-[(tert-
butyldimethylsilyl)oxy]ethyl](tert-butoxycarbonyl)amino]-3-
isopropoxyphenyl]amino]methyl]-4-(hydroxymethyl)-6-
isopropoxyphenyl]propanoic acid ethyl ester
                                             897644-39-2P, Ethyl
2-[2-[[[2-[[[4-[(amino)(hydroxyimino)methyl]phenyl]amino]carbonyl]-4-
methylphenyl]amino]methyl]-4-[(tert-butyldimethylsilyl)oxy]-6-
                           897644-40-5P, Ethvl
isopropoxyphenoxy]acetate
[[4-[[2-[[[5-(acetoxymethy1)-2-[(tert-
butoxycarbonyl)methyl]phenyl]methyl]amino]-5-
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methylbenzoyl]amino]phenyl](imino)methyl]carbamate
                                                     897644-46-1P.
tert-Butyl 2-[4-[[2-[(tert-butoxycarbonyl)amino]ethanoyl]amino]-2-[[[4-
chloro-2-[[[4-[(amino)(hydroxyimino)methyl]phenyl]amino]carbonyl]phenyl]am
inolmethvll-6-isopropoxyphenoxylacetate 897644-50-7P, Ethvl
3-[4-(2-acetoxyacetylamino)-2-[[[2-[[[4-
[(amino)(hydroxyimino)methyl]phenyl]amino]carbonyl]-4-
methylphenyl]amino]methyl]-6-isopropoxyphenyl]propanoate 897644-51-8P,
tert-Butyl 2-[2-[[[2-[[[4-[[(tert-
butoxycarbonyl)amino|(imino)methyl|phenyl|amino|carbonyl|-4-
chlorophenyllaminolmethyll-6-ethoxyphenoxylacetate
tert-Butvl 2-[2-[[[2-[[[4-[[(tert-
butoxycarbonyl)amino](imino)methyl]phenyl]amino]carbonyl]-4-
chlorophenyl]amino]methyl]-6-[2-(methylamino)-2-oxoethoxy]phenoxy]acetate
897644-54-1P, Ethyl 2-[4-acetoxymethyl-2-[[[2-[[[4-[[(tert-
butoxycarbonyl)amino](imino)methyl]phenyl]amino]carbonyl]-4-
methylphenyl]amino]methyl]-6-propoxyphenoxy]acetate 897644-55-2P,
N-[2-[[[2-[[[4-[[(tert-Butoxycarbonyl)amino](imino)methyl]phenyl]amino]car
bonyl]-4-chlorophenyl]amino]methyl]phenyl]-N-methylglycine
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
   (intermediate; preparation of carboxylic acid derivs. having three cyclic
   moieties as activated blood coagulation factor VII inhibitors and
   anticoaqulants)
897631-81-1P, tert-Butvl 2-[2-[[[2-[[[4-[[(tert-
butoxycarbonyl)amino](imino)methyl]phenyl]amino]carbonyl]-4-
chlorophenyl]amino|methyl]-6-hydroxyphenoxy|acetate 897631-88-8P,
tert-Butyl 2-[2-[[[2-[[[6-[amino(imino)methyl]pyridin-3-yl]amino]carbonyl]-
4-chlorophenvllamino|methvll-6-ethoxyphenoxylacetate formate
897632-09-6P, [3-[[[2-[[[4-[[(tert-
Butoxycarbonyl)amino](imino)methyl]phenyl]amino]carbonyl]-4-
chlorophenyl]amino]methyl]-2-(2-tert-butoxy-2-oxoethoxy)phenoxy]acetic
     897632-62-1P 897632-74-5P
                                   897632-78-9P 897632-85-8P
acid
897632-89-2P
              897632-95-0P 897639-97-3P 897640-72-1P
                                                           897640-75-4P
897641-61-1P
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic
preparation); THU (Therapeutic use); BIOL (Biological study); PREP
(Preparation); RACT (Reactant or reagent); USES (Uses)
   (preparation of carboxylic acid derivs. having three cyclic moieties as
   activated blood coagulation factor VII inhibitors and anticoagulants)
897631-80-0P, tert-Butvl 2-[2-[[[2-[[[4-[[(tert-
butoxycarbonyl)aminol(imino)methyllphenyllaminolcarbonyll-4-
cyanophenyl]amino]methyl]-6-ethoxyphenoxy]acetate 897631-82-2P,
tert-Butyl 2-[2-[[[2-[[[4-[[(tert-
butoxycarbonyl)amino](imino)methyl]phenyl]amino]carbonyl]-4-
chlorophenyl]amino]methyl]-6-[(1-methylpyrrolidin-2-
                            897631-83-3P, tert-Butvl
vl)methoxv|phenoxv|acetate
2-[4-amino-2-[[[2-[[[4-[[(tert-
butoxycarbonyl)aminol(imino)methyllphenyllaminolcarbonyll-4-
chlorophenyl]amino]methyl]-6-methoxyphenoxy]acetate
                                                     897631-84-4P, Ethvl
2-[2-[[[2-[[4-[amino(imino)methyl]benzoyl]amino]-4-
chlorophenyl]amino]methyl]-6-ethoxyphenoxy]acetate 897631-85-5P,
tert-Butyl 2-[2-[[[2-[[[4-[[(tert-
butoxycarbonyl)amino|(imino)methyl|phenyl|amino|carbonyl|-4-
chlorophenvllamino|methvll-4-chloro-6-(4-methvl-2-oxopiperazin-1-
yl)phenoxy]acetate 897631-86-6P, Ethyl
2-[2-[[[2-[[[4-[(amino)(hydroxyimino)methyl]phenyl]amino]carbonyl]-4-
chlorophenyl]amino]methyl]-6-ethoxyphenoxy]acetate
                                                   897631-90-2P,
tert-Butyl 2-[2-[[[2-[[[6-[amino(imino)methyl]pyridin-3-
yl]amino]carbonyl]phenyl]amino]methyl]-6-ethoxyphenoxy]acetate
        897631-91-3P, tert-Butyl
formate
2-[2-[[[2-[[[4-[amino(imino)methyl]phenyl]amino]carbonyl]-4-
chlorophenyl]amino]methyl]phenoxy]acetate 897631-92-4P, Ethyl
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3-[2-[[[2-[[[4-[(amino)(hydroxyimino)methyl]phenyl]amino]carbonyl]-4-
chlorophenyl]amino]methyl]piperidin-1-yl]propanoate
[2-[[2-[[4-[Amino(imino)methy1]pheny1]amino]carbony1]-4-
chlorophenvllaminolmethyllphenoxylacetic acid trifluoroacetate
897631-95-7P, [2-[[[2-[[[4-[Amino(imino)methyl]phenyl]amino]carbonyl]-4-
chlorophenyl]amino]methyl]-6-[2-(dimethylamino)ethoxy]phenoxy]acetic acid
hydrochloride
               897631-97-9P, [2-[[[2-[[[4-
[Amino(imino)methyl]phenyl]amino]carbonyl]-4-chlorophenyl]amino]methyl]-6-
[(3-methyloxetan-3-yl)methoxylphenoxylacetic acid trifluoroacetate
897631-98-0P, [2-[[[2-[[[4-(Aminomethyl)phenyl]amino]carbonyl]-4-
chlorophenyl]amino]methyl]-6-ethoxyphenoxy]acetic acid hydrochloride
897631-99-1P, [[3-[[[2-[[(2-Amino-1H-benzimidazo1-5-y1)amino|carbonv1]-4-
chlorophenyl]amino]methyl]biphenyl-2-yl]oxy]acetic acid 897632-01-8P,
4-[2-[[[2-[[[4-[Amino(imino)methyl]phenyl]amino]carbonyl]-4-
chlorophenyl]amino]methyl]piperidin-1-yl]butyric acid formate
897632-03-0P, 3-[2-[[[2-[[[4-[Amino(imino)methyl]phenyl]amino]carbonyl]-4-
chlorophenyl]amino]methyl]piperidin-1-yl]propanoic acid formate
897632-04-1P, [2-[1-[[2-[[[4-(Aminomethyl)phenyl]amino]carbonyl]-4-
chlorophenyl]amino]ethyl]phenoxy]acetic acid hydrochloride
                                                           897632-06-3P,
[2-[[[2-[[[6-[Amino(imino)methyl]pyridin-3-yl]amino]carbonyl]-4-
chlorophenyl|amino|methyl|-6-ethoxyphenoxy|acetic acid trifluoroacetate
897632-08-5P, [2-[[[2-[[[4-[Amino(imino)methyl]phenyl]amino]carbonyl]-4-
chlorophenyllaminolmethyll-6-(aminomethyl)phenoxylacetic acid
trifluoroacetate
                 897632-10-9P, tert-Butvl
2-[2-[[[2-[[[4-[[(tert-butoxycarbonyl)amino](imino)methyl]phenyl]amino]car
bonyl]-4-chlorophenyl]amino]methyl]-4-[[[(tert-
butoxycarbonyl)amino]sulfonyl]amino]-6-isopropoxyphenoxy]acetate
897632-12-1P, 3-[[[4-[Amino(imino)methyl]phenyl]amino]carbonyl]-4-[[2-(2-
carboxyethoxy)-3-ethoxybenzyl]amino]benzoic acid formate
897632-13-2P, [2-[[[2-[[[4-[Amino(imino)methyl]phenyl]amino]carbonyl]-4-
chlorophenyl]amino]methyl]-6-ethoxy-4-[(2-
hydroxyethyl) (methyl) amino]phenoxy]acetic acid hydrochloride
897632-14-3P, [2-||[2-||[4-|Amino(imino)methyl]phenyl]amino[carbonyl]-4-
methoxyphenyl]amino]methyl]-4-(hydroxymethyl)-6-isopropoxyphenoxy]acetic
      897632-15-4P, [2-[[[2-[[[4-
[Amino(imino)methyl]phenyl]amino]carbonyl]-4-chlorophenyl]amino]methyl]-4-
((1R)-1,2-dihydroxyethyl)-6-ethoxyphenoxy]acetic acid 897632-16-5P,
Ethyl 3-[2-[[[3-[[[4-[[(ethoxycarbonyl)amino](imino)methyl]phenyl]amino]ca
rbonyl]-5-methylpyridin-2-yl]amino]methyl]-4-(hydroxymethyl)-6-
isopropoxyphenyl|propanoate 897632-18-7P,
3-[2-[[[2-[[[2-[Amino(imino)methyl]pyrimidin-5-yl]amino]carbonyl]-4-
methylphenyllamino|methyl|-4-(hydroxymethyl)-6-isopropoxyphenyl|propanoic
acid formate
              897632-20-1P.
[2-[[[2-[[[4-[Amino(imino)methyl]phenyl]amino]carbonyl]-4-
methylphenyl]amino]methyl]-4-hydroxy-6-isopropoxyphenoxy]acetic acid
          897632-22-3P, [2-|||2-|||4-
formate
[Amino(imino)methyl]phenyl]amino[carbonyl]-4-methylphenyl]amino[methyl]-4-
(hydroxymethyl)-6-(2-hydroxy-1-methylethoxy)phenoxylacetic acid
          897632-24-5P, [2-[[[2-[[[4-
[Amino(imino)methyl]phenyl]amino]carbonyl]-4-methylphenyl]amino]methyl]-4-
(hydroxymethyl)phenoxy]acetic acid formate
                                            897632-25-6P,
[[2-[[[2-[[[4-[Amino(imino)methyl]phenyl]amino]carbonyl]-4-
chlorophenvllamino|methvll-6-methoxyphenvllamino|acetic acid
897632-27-8P, Ethyl 3-[2-[[[2-[[[4-
[amino(imino)methyl]phenyl]amino]carbonyl]-4-methylphenyl]amino]methyl]-4-
(hydroxymethyl)-6-isopropoxyphenyl]propanoate formate
897632-28-9P, 3-[2-[[[3-[[[4-[Amino(imino)methyl]phenyl]amino]carbonyl]-5-
methylpyridin-2-v1|amino|methyl|-4-(hydroxymethyl)-6-
isopropoxyphenyl]propanoic acid hydrochloride
                                               897632-30-3P,
3-[2-[[[2-[[[4-[Amino(imino)methyl]phenyl]amino]carbonyl]-4-
methylphenyl]amino]methyl]-4-(2-hydroxyethylamino)-6-
isopropoxyphenyl]propanoic acid formate 897632-31-4P,
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[2-[[3-[[4-[Amino(imino)methyl]phenyl]amino]carbonyl]pyridin-2-
v1|amino|methv1|-6-ethoxv-4-(hvdroxymethv1)phenoxy|acetic acid
hydrochloride
               897632-32-5P, Ethvl
2-[2-[[[2-[[[4-[(amino)(hydroxvimino)methyl]phenyl]amino]carbonyl]-4-
chlorophenyllaminolmethyll-4-(hydroxymethyl)-6-isopropoxyphenoxylacetate
              897632-33-6P, Methyl
hydrochloride
2-[2-[[[2-[[[4-[(amino)(hydroxyimino)methyl]phenyl]amino]carbonyl]-4-
methylphenyllamino|methyll-4-hydroxymethyl-6-isopropoxyphenoxylacetate
hvdrochloride
              897632-34-7P, Ethvl
2-[2-[[[2-[[[4-[(amino)(hydroxyimino)methyl]phenyl]amino]carbonyl]-4-
methylphenyllaminolmethyll-4-hydroxy-6-isopropoxyphenoxylacetate
897632-35-8P, Ethyl 2-[2-[[[2-[[[6-[(amino)(hydroxyimino)methyl]pvridin-3-
yl]amino]carbonyl]phenyl]amino]methyl]-4-hydroxymethyl-6-
isopropoxyphenoxylacetate 897632-36-9P,
[2-[[[2-[[]4-[[(Ethoxycarbonyl)amino](imino)methyl]phenyl]amino]carbonyl]-
4-methylphenyl]amino]methyl]-4-(hydroxymethyl)-6-isopropoxyphenyl]acetic
       897632-37-0P, 3-[[[2-[[[4-
[Amino(imino)methyl]phenyl]amino]carbonyl]-4-chlorophenyl]amino]methyl]-4-
(carboxymethoxy)-5-ethoxybenzoic acid hydrochloride 897632-38-1P, Ethyl
2-[2-[[[2-[[[4-[(amino)(hydroxyimino)methyl]phenyl]amino]carbonyl]-4-
fluorophenvl|amino|methvl|-4-(hydroxymethvl)-6-isopropoxyphenoxy|acetate
897632-39-2P, Ethvl 3-[2-[[[3-[[[4-
[[(ethoxycarbonyl)amino](imino)methyl]phenyl]amino]carbonyl]pyridin-2-
vllamino|methvll-4-(hydroxymethvl)-6-isopropoxyphenvl|propanoate
897632-40-5P, Ethyl 2-[2-[[[2-[[[6-[(amino)(hydroxyimino)methyl]pyridin-3-
v1]amino[carbonyl]-4-methylphenyl]amino[methyl]-4-(hydroxymethyl)-6-
isopropoxyphenoxylacetate hydrochloride 897632-41-6P, Ethyl
3-[2-[[[3-[[[4-[(amino)(hydroxyimino)methyl]phenyl]amino]carbonyl]-5-
methylpyridin-2-vllaminolmethyll-4-(hydroxymethyl)-6-
isopropoxyphenyl]propanoate hydrochloride 897632-42-7P,
N-[4-[(Amino)(hydroxyimino)methyl]phenyl]-2-[[2-[2-[(2-
hydroxyethyl) (methyl) amino]-2-oxoethoxy]-5-(hydroxymethyl)-3-
isopropoxybenzyl|amino|-5-methylbenzamide 897632-43-8P,
3-[2-[[[2-[[[4-[[(Ethoxycarbonyl)amino](imino)methyl]phenyl]amino]carbonyl
1-4-methylphenyllaminolmethyll-4-(hydroxymethyl)-6-
isopropoxyphenyl]propanoic acid
                                 897632-44-9P.
[2-[[[2-[[[4-[(Amino)(hydroxyimino)methyl]phenyl]amino]carbonyl]-4-
chlorophenyl]amino]methyl]-4-(glycylamino)-6-isopropoxyphenoxy]acetic acid
hydrochloride
               897632-46-1P, 3-[4-(2-Aminoacetylamino)-2-[[[2-[[[4-
[(amino)(hydroxyimino)methyl]phenyl]amino]carbonyl]-4-
methylphenyllamino|methyl|-6-isopropoxyphenyl|propanoic acid
trifluoroacetate
                  897632-47-2P, Ethvl
3-[4-(2-hydroxyacetylamino)-2-[[[2-[[[4-
[(amino)(hydroxyimino)methyl]phenyl]amino]carbonyl]-4-
methylphenyl]amino]methyl]-6-isopropoxyphenyl]propanoate
                                                          897632-48-3P.
3-[2-[[[2-[[[4-[(Amino)(hydroxyimino)methyl]phenyl]amino]carbonyl]-4-
methylphenyl|amino|methyl|-4-(hydroxymethyl)-6-isopropoxyphenyl|propanoic
                  897632-50-7P, [2-[[[2-[[[4-
acid sodium salt
[Amino(imino)methyl]phenyl]amino[carbonyl]-4-chlorophenyl]amino[methyl]-6-
ethoxyphenoxy]acetic acid trifluoroacetate
                                            897632-52-9P.
[2-[[[2-[[[4-[Amino(imino)methyl]phenyl]amino]carbonyl]-4-
methylphenyl[amino]methyl]-6-hydroxyphenoxy[acetic acid formate
897632-54-1P, [2-[[[2-[[[4-[Amino(imino)methyl]phenyl]amino]carbonyl]-4-
chlorophenv1]amino]methv1]-6-[2-(methvlamino)-2-oxoethoxy]phenoxy]acetic
acid formate
              897632-55-2P.
[2-[[[2-[[[4-[Amino(imino)methyl]phenyl]amino]carbonyl]-4-
chlorophenyl]amino]methyl]-4-[(dimethylamino)methyl]-6-
ethoxyphenoxy]acetic acid hydrochloride
                                         897632-57-4P,
[2-[[2-[[4-[Amino(imino)methyl]phenyl]amino]carbonyl]-4-
methylphenyl]amino]methyl]-4-(hydroxymethyl)-6-propoxyphenoxy]acetic acid
trifluoroacetate
                 897632-59-6P, [[2-[[[2-[[[4-
[Amino(imino)methyl]phenyl]amino]carbonyl]-4-
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chlorophenyl]amino]methyl]phenyl](methyl)amino]acetic acid formate
897632-61-0P, [2-[[[3-[[[4-[Amino(imino)methy1]pheny1]amino]carbony1]-2-
naphthyllamino|methyll-4-(hydroxymethyl)-6-isopropoxyphenoxylacetic acid
          897632-63-2P
                         897632-64-3P
                                         897632-65-4P
formate
897632-66-5P
               897632-67-6P
                              897632-68-7P
                                              897632-69-8P
                                                             897632-70-1P
897632-71-2P
               897632-72-3P
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897632-77-8P
               897632-79-0P
                              897632-80-3P
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897632-83-6P
               897632-84-7P
                              897632-86-9P
                                              897632-87-0P
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               897632-91-6P
                              897632-92-7P
                                              897632-93-8P
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897632-97-2P
               897632-99-4P
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                                              897633-03-3P
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897633-05-5P
               897633-06-6P
                              897633-07-7P
                                              897633-08-8P
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897633-10-2P
               897633-12-4P
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897633-16-8P
               897633-17-9P
                              897633-18-0P
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897633-21-5P
               897633-22-6P
                              897633-24-8P
                                              897633-26-0P
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897633-30-6P
               897633-32-8P
                              897633-34-0P
                                              897633-36-2P
                                                             897633-38-4P
897633-40-8P
               897633-42-0P
                              897633-44-2P
                                              897633-46-4P
                                                             897633-48-6P
897633-50-0P
               897633-52-2P
                              897633-54-4P
                                              897633-56-6P
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897633-60-2P
               897633-62-4P
                              897633-64-6P
                                              897633-66-8P
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897633-70-4P
               897633-72-6P
                              897633-74-8P
                                                             897633-78-2P
897633-80-6P
               897633-82-8P
                              897633-84-0P
                                              897633-86-2P
                                                             897633-88-4P
897633-90-8P
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                              897633-94-2P
                                              897633-96-4P
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897633-98-6P
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                                              897634-01-4P
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897634-03-6P
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897634-71-8P
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897634-91-2P
               897634-93-4P
                              897634-95-6P
                                              897634-97-8P
                                                             897634-99-0P
897635-01-7P
              897635-03-9P
                              897635-04-0P
                                             897635-05-1P
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897635-08-4P
              897635-10-8P
                              897635-12-0P
                                             897635-14-2P
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897635-17-5P
                                             897635-23-3P
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               897635-19-7P
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897635-26-6P
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                                              897635-31-3P
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897635-43-7P
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897635-49-3P
               897635-50-6P
                              897635-51-7P
                                             897635-52-8P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
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(Uses) (preparation of carboxylic acid derivs. having three cyclic moieties as activated blood coagulation factor VII inhibitors and anticoagulants) 897635-53-9P 897635-55-1P 897635-56-2P 897635-57-3P 897635-58-4P 897635-59-5P 897635-61-9P 897635-62-0P 897635-64-2P 897635-66-4P 897635-67-5P 897635-69-7P 897635-71-1P 897635-73-3P 897635-75-5P 897635-76-6P 897635-78-8P 897635-79-9P 897635-81-3P 897635-83-5P 897635-85-7P 897635-87-9P 897635-89-1P 897635-91-5P 897635-93-7P 897635-95-9P 897635-97-1P 897635-99-3P 897636-01-0P 897636-03-2P 897636-05-4P 897636-07-6P 897636-12-3P 897636-14-5P 897636-09-8P 897636-16-7P 897636-18-9P 897636-20-3P 897636-22-5P 897636-24-7P 897636-29-2P 897636-31-6P 897636-26-9P 897636-27-0P 897636-28-1P 897636-33-8P 897636-35-0P 897636-37-2P 897636-39-4P 897636-41-8P 897636-42-9P 897636-43-0P 897636-45-2P 897636-47-4P 897636-49-6P 897636-51-0P 897636-53-2P 897636-55-4P 897636-56-5P. [2-[[[2-[[[4-[Amino(imino)methyl]phenyl]amino]carbonyl]-4chlorophenyl[amino]methyl]-4-[(aminosulfonyl)amino]-6isopropoxyphenoxy]acetic acid 897636-57-6P 897636-59-8P 897636-60-1P 897636-61-2P 897636-63-4P 897636-65-6P 897636-67-8P 897636-69-0P 897636-77-0P

897636-75-8P

897636-80-5P

897636-76-9P

897636-83-8P

897636-81-6P

897636-71-4P

897636-78-1P

897636-73-6P

897636-79-2P

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             897636-94-1P
                             897636-96-3P
                                           897636-97-4P
                                                          897636-99-6P
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            897637-33-1P
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897637-41-1P 897637-43-3P
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897638-16-3P
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897638-23-2P
             897638-25-4P
                            897638-26-5P
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                            897638-63-0P
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897638-68-5P
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                                           897638-72-1P
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897638-75-4P
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                             897638-79-8P
                                           897638-81-2P
                                                          897638-83-4P
897638-85-6P
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                             897638-89-0P
                                            897638-91-4P
                                                          897638-93-6P
897638-95-8P
              897638-97-0P
                             897638-99-2P
                                            897639-01-9P
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897639-05-3P
              897639-07-5P
                             897639-09-7P
                                           897639-11-1P
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897639-14-4P
              897639-16-6P
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                                                          897639-23-5P
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897639-25-7P
              897639-27-9P
                             897639-29-1P
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897639-34-8P
             897639-36-0P
                            897639-38-2P
                                           897639-40-6P
                                                          897639-41-7P
897639-43-9P
             897639-44-0P
                            897639-45-1P
                                           897639-46-2P
                                                          897639-47-3P
             897639-50-8P
                            897639-52-0P
                                           897639-54-2P
                                                          897639-56-4P
897639-48-4P
897639-57-5P
              897639-58-6P
                            897639-59-7P
                                          897639-61-1P
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897639-63-3P
             897639-65-5P
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RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES

(preparation of carboxylic acid derivs. having three cyclic moieties as

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activated blood coagulation factor VII inhibitors and anticoagulants)
897639-66-6P 897639-67-7P 897639-68-8P 897639-69-9P 897639-71-3P
897639-73-5P
            897639-75-7P 897639-77-9P
                                         897639-79-1P
                                                        897639-81-5P
897639-82-6P 897639-83-7P 897639-84-8P 897639-85-9P 897639-86-0P
897639-87-1P 897639-88-2P 897639-89-3P 897639-90-6P 897639-91-7P
897639-92-8P 897639-93-9P 897639-94-0P 897639-95-1P 897639-96-2P
897639-98-4P 897639-99-5P 897640-00-5P 897640-01-6P 897640-02-7P
897640-03-8P 897640-04-9P 897640-05-0P 897640-06-1P 897640-07-2P
897640-08-3P 897640-09-4P
                           897640-10-7P
                                         897640-11-8P
                                                        897640-12-9P
897640-13-0P
            897640-14-1P
                           897640-15-2P
                                         897640-16-3P
                                                        897640-17-4P
897640-18-5P
            897640-19-6P
                           897640-20-9P
                                         897640-21-0P
                                                        897640-22-1P
897640-23-2P
                                         897640-27-6P
            897640-25-4P
                           897640-26-5P
                                                        897640-28-7P
897640-29-8P
              897640-30-1P
                            897640-31-2P
                                          897640-32-3P
                                                        897640-34-5P
897640-35-6P
              897640-36-7P
                            897640-38-9P
                                          897640-39-0P
                                                        897640-41-4P
897640-42-5P
              897640-43-6P
                            897640-44-7P
                                          897640-45-8P
                                                         897640-47-0P
897640-48-1P
             897640-49-2P
                            897640-50-5P
                                          897640-51-6P
                                                         897640-52-7P
                                          897640-56-1P
897640-53-8P
              897640-54-9P
                            897640-55-0P
                                                         897640-57-2P
897640-58-3P
              897640-59-4P
                            897640-60-7P
                                          897640-61-8P
                                                         897640-62-9P
897640-63-0P
              897640-64-1P
                            897640-65-2P
                                          897640-66-3P
                                                         897640-67-4P
897640-68-5P
              897640-69-6P
                            897640-70-9P
                                          897640-71-0P
                                                         897640-73-2P
897640-74-3P
             897640-77-6P
                            897640-78-7P
                                          897640-79-8P
                                                         897640-80-1P
897640-81-2P
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                            897640-83-4P
                                          897640-84-5P
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897640-86-7P
             897640-87-8P
                            897640-88-9P
                                          897640-89-0P
                                                         897640-90-3P
                                                         897640-95-8P
897640-91-4P
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897640-96-9P
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897641-05-3P

897641-01-9P

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897641-12-2P 897641-13-3P 897641-14-4P 897641-15-5P 897641-16-6P
897641 - 17 - 7P \qquad 897641 - 18 - 8P \qquad 897641 - 19 - 9P \qquad 897641 - 21 - 3P \qquad 897641 - 22 - 4P \qquad 897641 - 21 - 3P \qquad 897641 - 22 - 4P \qquad 897641 - 21 - 3P \qquad 897641 - 22 - 4P \qquad 897641 - 21 - 3P \qquad 897641 - 21 - 3P \qquad 897641 - 22 - 4P \qquad 897641 - 21 - 3P \qquad 897641 - 21
897641-24-6P 897641-25-7P 897641-26-8P 897641-27-9P 897641-28-0P
897641-29-1P 897641-30-4P 897641-31-5P 897641-32-6P 897641-33-7P
897641-34-8P 897641-35-9P 897641-37-1P 897641-39-3P 897641-40-6P
897641-41-7P 897641-42-8P 897641-43-9P 897641-44-0P 897641-45-1P
897641-46-2P 897641-47-3P 897641-48-4P 897641-49-5P 897641-51-9P
897641-54-2P 897641-57-5P 897641-65-5P 897641-68-8P 897641-71-3P
897641-73-5P 897644-38-1P, Ethvl
2-[2-[[[2-[[[4-[(amino)(hydroxyimino)methyl]phenyl]amino]carbonyl]-4-
chlorophenyl]amino]methyl]-4-(hydroxymethyl)-6-isopropoxyphenoxy]acetate
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
(Uses)
     (preparation of carboxylic acid derivs. having three cyclic moieties as
     activated blood coagulation factor VII inhibitors and anticoagulants)
50-00-0, Formaldehyde, reactions 57-57-8, β-Propiolactone
75-03-6, Iodoethane 89-63-4, 4-Chloro-2-nitroaniline 90-02-8,
Salicylaldehyde, reactions 98-80-6, Phenylboronic acid 100-97-0,
Hexamethylenetetramine, reactions 107-21-1, Ethylene glycol, reactions 107-30-2, Chloromethyl methyl ether 108-01-0, 2-(Dimethylamino
)ethanol 108-16-7; 1-Dimethylamino-2-propanol 109-83-1, 2-(Methylamino)-propanol 109-83-1, 2-(Methylamino)-propanol 109-83-1, 2-(Methylamino)-propanol 109-83-1, 5-Filuorosalicylic acid 358-23-6, Trifluorosethanesulfonic acid anhydride
492-88-6, 3-Ethoxy-2-hydroxybenzaldehyde 541-41-3, Ethyl chloroformate
619-65-8, 4-Cyanobenzoic acid 635-21-2, 5-Chloroanthranilic acid
1125-88-8, Benzaldehyde dimethyl acetal 1484-84-0,
2-(Piperidin-2-yl)ethanol 1609-47-8, Diethyl dicarbonate
2498-50-2, 4-Aminobenzamidine dihydrochloride 2516-95-2,
5-Chloro-2-nitrobenzoic acid 3143-02-0, (3-Methyloxetan-3-y1)methanol
3433-37-2, Piperidin-2-ylmethanol 4421-08-3, 4-Cyano-2-methoxyphenol
4530-20-5, 2-(tert-Butoxycarbonylamino)acetic acid 4692-98-2,
5-Bromoisatoic anhydride 5274-70-4, 3-Nitrosalicylaldehyde
5330-38-1, 4-Chloro-2-(hydroxymethyl)phenol 5470-11-1 6092-54-2,
n-Hexyl chloroformate 6628-86-0, 5-Chloro-2-nitrobenzaldehyde
6630-33-7, 2-Bromobenzaldehyde 7486-35-3, Tributylvinyltin 10463-20-4,
(4-Hydroxy-3-nitrophenyl)acetic acid 18162-48-6,
tert-Butyldimethylchlorosilane 24424-99-5, Di-tert-butyl dicarbonate
24677-78-9, 2,3-Dihydroxybenzaldehyde 26908-34-9,
2-(1,3-Dioxolan-2-v1)aniline 27532-96-3, Glycine tert-butyl ester
hydrochloride
                        28539-02-8, 1H-Benzotriazole-1-methanol 30525-89-4,
Paraformaldehyde 34770-60-0, 4-Methylpiperazin-2-one 37585-25-4,
(2-Amino-5-chlorophenyl)methanol 51779-32-9, Di-tert-butyl
iminodicarboxylate 53055-05-3, 3-Methoxy-2-nitrobenzaldehyde
57018-52-7, 1-tert-Butoxy-2-propanol 67868-82-0,
3-(Methylsulfanyl)salicylaldehyde 71118-98-4,
4-Hydroxy-3-isopropoxybenzaldehyde 74786-02-0,
(1-tert-Butoxyvinyloxy) (tert-butyl)dimethylsilane 86734-60-3,
2-Benzyloxy-3-hydroxybenzaldehyde 94838-55-8, tert-Butyl
(4-aminobenzyl)carbamate 102191-92-4,
2-[(tert-Butyldimethylsilyl)oxy]acetaldehyde
                                                                            136088-69-2 147000-89-3,
N-(tert-Butoxycarbonyl)sulfamyl chloride 150655-06-4,
3-Ethoxy-2-hydroxy-5-nitrobenzaldehyde 155891-51-3.
2-(Bromomethyl)benzyl acetate 192130-58-8, Poly(ethyl glyoxylate)
222031-87-0, 2-Hydroxy-3-isopropoxybenzaldehyde 897640-67-4.
3-[2-[[[3-[[[4-[(Amino)(hydroxyimino)methyl]phenyl]amino]carbonyl]-5-
methylpyridin-2-yl]amino]methyl]-4-(hydroxymethyl)-6-
isopropoxyphenyl]propanoic acid hydrochloride 897643-91-3, tert-Butyl
2-(2-ethoxy-6-formyl-4-iodophenoxy)acetate 897643-94-6, tert-Butyl
3-(4-amino-2-hydroxymethyl-6-isopropoxyphenyl)propanoate 897644-14-3,
Ethyl 2-[4-[[4-[[(tert-butoxycarbonyl)amino](imino)methyl]phenyl]carbamoyl
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]-3-nitrophenyl]acetate
                        897644-16-5, Methanesulfonic acid
2-tert-butoxy-1-methylethyl ester 897644-17-6, tert-Butyl
3-[2-[[[2-[[[4-[(amino)(hydroxyimino)methyl]phenyl]amino]carbonyl]-4-
chlorophenyl]amino]methyl]piperidin-1-yl]propanoate
                                                  897644-18-7,
tert-Butyl 2-[2-[[[2-[[[4-[[(tert-
butoxycarbonyl)amino](imino)methyl]phenyl]amino]carbonyl]-4-
chlorophenyl]amino]methyl]phenoxy]acetate 897644-19-8, tert-Butyl
2-(2-acetylphenoxy)acetate 897644-23-4, tert-Butyl
2-[2-[(benzyloxycarbonyl)methoxy]-6-[[[2-[[[4-[[(tert-
butoxycarbonyl)aminol(imino)methyllphenyllaminolcarbonyll-4-
chlorophenyl]amino]methyl]phenoxy]acetate 897644-24-5, Methyl
3-[[4-[[(tert-butoxycarbonyl)amino](imino)methyl]phenyl]amino]carbonyl]-4-
[[2-(2-tert-butoxy-2-oxoethoxy)-3-ethoxybenzyl]amino]benzoate
897644-25-6, tert-Butyl 2-[4-((1R)-1,2-dihydroxyethyl)-2-ethoxy-6-
formylphenoxylacetate 897644-26-7, Ethyl
3-(4-acetoxymethyl-2-formyl-6-isopropoxyphenyl)propanoate 897644-27-8,
2-Amino-N-[2-[amino(imino)methyl]pyrimidin-5-yl]-5-methylbenzamide
hydrochloride 897644-31-4, Ethyl
2-[2-formyl-4-(hydroxymethyl)phenoxy]acetate
                                            897644-32-5, tert-Butyl
2-[(2-formyl-6-methoxyphenyl)(trifluoroacetyl)amino]acetate 897644-33-6,
2-Amino-N-[4-[amino(imino)methyl]phenyl]-5-methylbenzamide
                                                          897644-34-7,
Ethyl 3-[2-formyl-4-(hydroxymethyl)-6-isopropoxyphenyl]propanoate
897644-41-6, Methyl 4-(2-tert-butoxy-2-oxoethoxy)-3-ethoxy-5-
formylbenzoate 897644-43-8, Ethyl
2-[4-acetoxymethyl-2-[[[2-[[[4-
[(amino)(hydroxyimino)methyl]phenyl]amino]carbonyl]-4-
methylphenyl]amino]methyl]-6-isopropoxyphenoxy]acetate
                                                       897644-44-9.
tert-Butyl 3-[2-[[[2-[[[4-
[[(ethoxycarbonyl)amino](imino)methyl]phenyl]amino]carbonyl]-4-
methylphenyl]amino]methyl]-4-(hydroxymethyl)-6-isopropoxyphenyl]propanoate
897644-45-0, tert-Butyl 2-[4-amino-2-[[[4-chloro-2-[[[4-
[(amino)(hydroxyimino)methyl]phenyl]amino]carbonyl]phenyl]amino]methyl]-6-
isopropoxyphenoxy]acetate
                         897644-47-2, Ethyl
3-[4-[[N-(tert-butoxycarbonyl)glycyl]amino]-2-formyl-6-
isopropoxyphenyl]propanoate 897644-48-3, Ethyl
3-[4-[[2-(tert-butoxycarbonylamino)ethanoyl]amino]-2-[[[2-[[[4-
[(amino)(hydroxyimino)methyl]phenyl]amino]carbonyl]-4-
methylphenyl]amino]methyl]-6-isopropoxyphenyl]propanoate
Ethyl 3-[4-[(acetoxyacetyl)amino]-2-formyl-6-isopropoxyphenyl]propanoate
897644-53-0, Ethyl 2-(4-acetoxymethyl-2-formyl-6-propoxyphenoxy)acetate
RL: RCT (Reactant); RACT (Reactant or reagent)
   (preparation of carboxylic acid derivs. having three cyclic moieties as
   activated blood coagulation factor VII inhibitors and anticoagulants)
68007-03-4P 75372-00-8P
                         95202-37-2P 95202-38-3P
                                                    897642-53-4P
897642-54-5P 897642-55-6P 897642-56-7P 897642-57-8P
                                                         897642-58-9P
897642-59-0P 897642-60-3P 897642-61-4P
                                          897642-62-5P
                                                        897642-63-6P
897642-64-7P 897642-65-8P 897642-66-9P 897642-67-0P 897642-68-1P
897642-69-2P 897642-70-5P 897642-71-6P 897642-72-7P 897642-73-8P
897642-74-9P 897642-75-0P 897642-76-1P 897642-77-2P 897642-78-3P
897642-79-4P 897642-80-7P 897642-81-8P 897642-82-9P 897642-83-0P
897642-84-1P 897642-85-2P 897642-86-3P 897642-87-4P 897642-88-5P
897642-89-6P 897642-90-9P 897642-91-0P 897642-92-1P
                                                        897642-93-2P
                                          897642-97-6P
897642-94-3P
             897642-95-4P
                            897642-96-5P
                                                        897642-98-7P
                                          897643-02-6P
             897643-00-4P
                            897643-01-5P
                                                        897643-03-7P
897642-99-8P
             897643-05-9P
                            897643-06-0P
                                          897643-08-2P
                                                        897643-10-6P
897643-04-8P
897643-11-7P
             897643-12-8P
                            897643-13-9P
                                          897643-14-0P
                                                         897643-15-1P
897643-16-2P
             897643-17-3P
                            897643-18-4P
                                           897643-19-5P
                                                         897643-20-8P
897643-21-9P
             897643-22-0P
                            897643-23-1P 897643-24-2P
                                                         897643-25-3P
897643-26-4P 897643-27-5P
                            897643-28-6P 897643-29-7P
                                                         897643-30-0P
897643-31-1P 897643-32-2P
                            897643-33-3P 897643-34-4P
                                                         897643-35-5P
897643-36-6P 897643-37-7P 897643-38-8P 897643-39-9P 897643-40-2P
897643-41-3P 897643-42-4P 897643-43-5P 897643-44-6P
                                                         897643-45-7P
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897643-46-8P 897643-47-9P 897643-48-0P 897643-49-1P 897643-50-4P
897643-51-5P 897643-52-6P 897643-53-7P 897643-54-8P 897643-55-9P
897643-56-0P 897643-57-1P 897643-58-2P 897643-59-3P 897643-60-6P
897643-61-7P 897643-62-8P 897643-63-9P 897643-64-0P 897643-65-1P
897643-66-2P 897643-67-3P 897643-68-4P 897643-69-5P 897643-70-8P
897643-71-9P 897643-72-0P 897643-73-1P 897643-74-2P 897643-75-3P
897643-76-4P 897643-77-5P 897643-78-6P 897643-79-7P 897643-80-0P
897643-81-1P 897643-82-2P 897643-83-3P 897643-84-4P
                                                    897643-85-5P
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RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of carboxylic acid derivs. having three cyclic moieties as activated blood coagulation factor VII inhibitors and anticoagulants)

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897643-86-6P 897643-87-7P 897643-88-8P 897643-89-9P
RE.CNT 32
             THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE
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(2) Eisai Co Ltd; US 5716993 A 1996 CAPLUS
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(4) Eisai Co Ltd; WO 9518097 A1 1996 CAPLUS
(5) Eli Lilly And Co; EP 1019047 A1 2001 CAPLUS
(6) Eli Lilly And Co; JP 2001523256 A 2001
(7) Eli Lilly And Co; US 6541499 B1 2001 CAPLUS
(8) Eli Lilly And Co; WO 9848800 A1 2001 CAPLUS
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(10) Eli Lilly And Co; WO 2000039118 A1 2002
(11) Eli Lilly And Co; JP 2002533454 A 2002
(12) Eli Lilly And Co; US 6635657 B1 2002 CAPLUS
(13) Eli Lilly And Co; EP 1140881 A1 2004 CAPLUS
(14) Eli Lilly And Co; WO 2000039111 A1 2004
(15) Eli Lilly And Co; JP 2004522689 A 2004
(16) Eli Lilly And Co; US 6610704 B1 2004 CAPLUS
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(18) Japan Tobacco Inc; WO 2004020393 A1 2004 CAPLUS
(19) Japan Tobacco Inc; JP 2004323504 A 2004 CAPLUS
(20) Novartis Ag; EP 1259487 A1 2003 CAPLUS
(21) Novartis Ag; EP 1446381 Al 2003 CAPLUS
(22) Novartis Aq; WO 2001055114 A1 2003
(23) Novartis Aq; WO 2003040101 A1 2003
(24) Novartis Aq; JP 2003520853 A 2003
(25) Novartis Aq; JP 2005508382 A 2003
(26) Schering Ag; EP 1392680 A2 2004 CAPLUS
(27) Schering Ag: EP 1594841 A1 2004 CAPLUS
(28) Schering Ag: WO 2002090352 A2 2004 CAPLUS
(29) Schering Ag; WO 2004013102 A1 2004 CAPLUS
(30) Schering Ag; JP 2004528379 A 2004
(31) Schering Ag; JP 2005538112 A 2004
(32) Yamanouchi Pharmaceutical Co Ltd; JP 2004315395 A 2004 CAPLUS
L9
    ANSWER 13 OF 55 CAPLUS COPYRIGHT 2009 ACS on STN
AN
    2006:536488 CAPLUS
DN
     145:254490
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- ΕD Entered STN: 08 Jun 2006
- TΙ A vapour hazard index for use with COSHH and DSEAR
- Pitt, Martin J.
- CS Chemical and Process Engineering, University of Sheffield, UK
 - Institution of Chemical Engineers Symposium Series (2006), 151 (Hazards XIX: Process Safety and Environmental Protection -- What do we Know? Where are we Going?), 95-107
- CODEN: ICESDB; ISSN: 0307-0492
- PB Institution of Chemical Engineers
- DT Journal
- LA English

- CC 59-5 (Air Pollution and Industrial Hygiene) Section cross-reference(s): 4, 45
- For workers who may be exposed to chemical vapors, the Control of Substances Hazardous to Health Regulations 2002 (amended 2004) and Dangerous Substances and Explosive Atmospheres Regulations 2002 require risk assessment and control of the hazard. For example, if a solvent cleaning process is planned, the employer should review possible options and determine if workers may be exposed to an unsafe levels of harmful vapor. If so, steps must be taken to modify the work or protect the worker by ventilation, respiratory protection, etc. From Apr. 2005, Workplace Exposure Limits (WEL) replaced the former Occupational Exposure Stds. (OES) and Occupational Exposure Limits (OEL); however, these do not directly measure hazards because in practice, they are also determined by the amount of vapor emitted by a liquid, which depends on its vapor pressure. Thus, a Vapor Hazard Index is proposed and listed for volatile substances and gases with a WEL. This is the saturated vapor pressure: WEL ratio, i.e, the amount by which the vapor will exceed the WEL in a confined space. It combines the toxicol. standard and phys. properties and can be used for an initial risk assessment, e.g., to compare the danger of alternative solvents. It may also be used to specify control measures and is comparable with practice in other countries. For many users, it is suggested this may be more directly useful than the WEL, so it is proposed that the Vapor Hazard Index should be published along with WEL in the
- ST occupational health hazard vapor hazard index volatile substance gas; volatile substance gas vapor hazard index occupational safety

IT Health hazard

(gaseous; vapor hazard index to assess and control volatile substance and gas vapor hazards to ensure compliance with safety, health, and dangerous substances and explosive atmospheres regulations in UK)

IT Gases

(hazardous; vapor hazard index to assess and control volatile substance and gas vapor hazards to ensure compliance with safety, health, and dangerous substances and explosive atmospheres regulations in UK)

IT Standards, legal and permissive

(occupational safety; vapor hazard index to assess and control volatile substance and gas vapor hazards to ensure compliance with safety, health, and dangerous substances and explosive atmospheres regulations in UK)

T Explosibility

Uuman

Industrial hygiene

Occupational health hazard

Occupational safety

Risk assessment

Volatile substances

(vapor hazard index to assess and control volatile substance and gas vapor hazards to ensure compliance with safety, health, and dangerous substances and explosive atmospheres regulations in UK)

IT Turpentine

RL: ADV (Adverse effect, including toxicity); PRP (Properties); TEM (Technical or engineered material use); BIOL (Biological study); USES (Uses)

(vapor hazard index to assess and control volatile substance and gas vapor hazards to ensure compliance with safety, health, and dangerous substances and explosive atmospheres regulations in UK)

IT Air pollution

Indoor air pollution

(workplace air, vapor hazard index to assess and control volatile substance and gas vapor hazards to ensure compliance with safety, health, and dangerous substances and explosive atmospheres regulations in UK) IT 50-00-0, Formaldehyde, biological studies 56-23-5, Carbon tetrachloride, biological studies 60-29-7, Diethyl ether, biological studies Aniline, biological studies 64-17-5, Ethanol, biological studies 64-18-6, Formic acid, biological studies 64-67-5, Diethylsulfate 67-56-1, Methanol, biological studies 67-63-0, 2-Propanol, biological studies 67-64-1, Acetone, biological studies 67-66-3, Chloroform, biological studies 68-12-2, Dimethylformamide, biological studies 71-23-8, 1-Propanol, biological studies 71-43-2, Benzene, biological studies 71-55-6, 1,1,1-Trichloroethane 74-83-9, Bromomethane, biological studies 74-87-3, Chloromethane, biological studies 74-90-8, Hydrogen cyanide, biological studies 74-93-1, Methanethiol, biological studies 75-00-3, Chloroethane 75-01-4, Vinyl chloride, biological studies 75-04-7, Ethylamine, biological studies 75-05-8, Acetonitrile, biological studies 75-07-0, Acetaldehyde, biological studies 75-08-1, Ethanethiol 75-09-2, Dichloromethane, biological studies 75-15-0, Carbon disulfide, biological studies 75-21-8, Ethylene oxide, biological studies 75-34-3, 1,1-Dichloroethane 75-35-4, Vinylidene chloride, biological studies 75-43-4, Dichlorofluoromethane 75-44-5, Phosgene 75-45-6, Chlorodifluoromethane 75-52-5, Nitromethane, biological studies 75-56-9, Propylene oxide, biological studies 75-65-0, 2-Methylpropan-2-ol, biological studies 76-06-2, Trichloronitromethane 77-78-1, Dimethylsulfate 78-83-1, 2-Methylpropan-1-ol, biological studies 78-92-2, 2-Butanol 78-93-3, 2-Butanone, biological studies 79-01-6, Trichloroethylene, biological studies 79-09-4, Propionic acid, biological studies 79-20-9, Methylacetate 79-27-6, 1,1,2,2-Tetrabromoethane 79-46-9, 2-Nitropropane 80-62-6, Methyl methacrylate 95-47-6, o-Xylene, biological studies 95-50-1, 1,2-Dichlorobenzene 95-53-4, o-Toluidine, biological studies 96-22-0, 3-Pentanone 98-01-1, 2-Furaldehyde, biological studies 98-82-8, Cumene 98-95-3, Nitrobenzene, biological 100-41-4, Ethylbenzene, biological studies 100-42-5, Styrene, biological studies 100-44-7, Benzyl chloride, biological studies 100-61-8, N-Methylaniline, biological studies 100-74-3, 4-Ethylmorpholine 101-84-8, Diphenyl ether 106-35-4, 3-Heptanone 106-42-3, p-Xylene, biological studies 106-46-7, 1,4-Dichlorobenzene 106-93-4, Ethylene dibromide 107-02-8, Acrolein, biological studies 107-06-2, Ethylene dichloride, biological studies 107-13-1, Acrylonitrile, biological studies 107-18-6, Allyl alcohol, biological 107-19-7, 2-Propyn-1-ol 107-87-9, 2-Pentanone 107-98-2, 1-Methoxypropan-2-ol 108-01-0, 2-Dimethylaminoethanol 108-10-1, 4-Methylpentan-2-one 108-18-9, Diisopropylamine 108-20-3, Diisopropyl ether 108-23-6, Isopropyl chloroformate 108-24-7, Acetic anhydride 108-38-3, m-Xylene, biological studies 108-83-8, 2,6-Dimethylheptan-4-one 108-88-3, Toluene, biological studies 108-90-7, Chlorobenzene, biological studies 108-91-8, Cyclohexylamine, biological studies 108-93-0, Cyclohexanol, biological studies 108-94-1, Cyclohexanone, biological studies 109-60-4, n-Propyl acetate 109-86-4, 2-Methoxyethanol 109-87-5, Dimethoxymethane 109-89-7, Diethylamine, biological studies 109-94-4, Ethylformate 109-99-9, Tetrahydrofuran, biological studies 110-12-3, 5-Methylhexan-2-one 110-19-0, Isobutyl acetate 110-43-0, 2-Heptanone 110-49-6, 2-Methoxyethyl acetate 110-54-3, n-Hexane, biological studies 110-80-5, 2-Ethoxyethanol 110-82-7, Cyclohexane, biological studies 110-86-1, Pyridine, biological studies 110-89-4, Piperidine, biological studies 111-15-9, 2-Ethoxyethyl acetate 111-30-8, Glutaraldehyde 111-76-2, 2-Butoxyethanol 112-07-2, 2-Butoxyethyl acetate 115-10-6, Dimethyl ether 120-82-1, 1,2,4-Trichlorobenzene 121-44-8, Triethylamine, biological studies 123-51-3, 3-Methylbutan-1-ol 123-86-4, n-Butyl acetate 123-91-1, 1,4-Dioxane, biological studies

124-38-9, Carbon dioxide, biological studies 124-40-3, Dimethylamine, biological studies 127-18-4, Tetrachloroethylene, biological studies 127-19-5, N,N-Dimethylacetamide 138-22-7, Butyl lactate 140-88-5,

Ethyl acrylate 141-43-5, 2-Aminoethanol, biological studies 141-78-6, Ethyl acetate, biological studies 142-82-5, n-Heptane, biological studies 151-67-7, Halothane 156-59-2, cis-1,2-Dichloroethylene 156-60-5, trans-1,2-Dichloroethylene 302-01-2, Hydrazine, biological studies 463-51-4, Ketene 541-41-3, Ethyl chloroformate 541-85-5, 5-Methylheptan-3-one 542-88-1, Bis(chloromethyl ether) 583-60-8, 2-Methylcyclohexanone 591-78-6, 2-Hexanone 628-63-7, Pentyl acetate 630-08-0, Carbon monoxide, biological studies 811-97-2, 1,1,1,2-Tetrafluoroethane 872-50-4, 1-Methvl-2-pyrrolidone, biological studies 1634-04-4, Methyl-tert-butyl ether 2551-62-4, Sulfur hexafluoride 2699-79-8, Sulfuryl difluoride 7647-01-0, Hydrogen chloride, biological studies 7664-39-3, Hydrogen fluoride, biological studies 7664-41-7, Ammonia, biological studies 7726-95-6, Bromine, biological studies 7782-41-4, Fluorine, biological studies 7782-50-5, Chlorine, biological studies 7782-65-2, Germane 7783-06-4, Hydrogen sulfide, biological studies 7784-42-1, Arsine 7803-51-2, Phosphine 7803-62-5, Silane, biological studies 10024-97-2, Nitrous oxide, biological studies 10025-87-3, Phosphoryl trichloride 10035-10-6, Hydrogen bromide, biological studies 10049-04-4, Chlorine dioxide 25154-54-5, Dinitrobenzene 25551-13-7, Trimethylbenzene 25639-42-3, Methylcyclohexanol 26952-21-6, Isooctyl alcohol 86475-92-5, 1-Methoxypropylacetate RL: ADV (Adverse effect, including toxicity); PRP (Properties); TEM

(Technical or engineered material use); BIOL (Biological study); USES (USES) (vapor hazard index to assess and control volatile substance and gas vapor hazards to ensure compliance with safety, health, and dangerous

substances and explosive atmospheres regulations in UK)
RE.CNT 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD

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- http://www.jtbaker.com/asp/catalog.asp
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- (16) Wypych, G; Knovel Solvents -- A Properties Database 2000
- L9 ANSWER 14 OF 55 CAPLUS COPYRIGHT 2009 ACS on STN
- AN 2006:137980 CAPLUS
- DN 144:192505
- ED Entered STN: 15 Feb 2006

- TI Method for preparation of Zofenopril for treating hypertension
- IN Zhang, Fuli; An, Dong; Pan, Linyu; Xie, Meihua
- PA Shanghai Institute of Pharmaceutical Industry, Peop. Rep. China; Jiangsu Kanion Pharmaceutical Co., Ltd.
- SO Faming Zhuanli Shenqing Gongkai Shuomingshu, 15 pp.
- CODEN: CNXXEV
- DT Patent LA Chinese
- LA Chinese IC ICM C07D207-16
- ICS A61P009-12
- CC 34-2 (Amino Acids, Peptides, and Proteins) Section cross-reference(s): 1

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PΙ	CN 1594291	A	20050316	CN 2003-150893	20030910
	CN 1245383	C	20060315		
PRAI	CN 2003-150893		20030910		

CLASS

- PATENT NO. CLASS PATENT FAMILY CLASSIFICATION CODES

 ON 1594291 ICM C07D207-16
 - ICS A61P009-12 IPCI C07D0207-00
 - IPCI C07D0207-00 [I,C]; C07D0207-16 [I,A]
 IPCR A61P0009-00 [I,C*]; A61P0009-12 [I,A]; C07D0207-00
 [I,C*]; C07D0207-16 [I,A]
- OS CASREACT 144:192505
- AB The method comprises acylating (R,S)-3-benzoylthio-2-Me propanoic acid with acylation agent such as SCC12, PCl3, PCl3, PCC13 at -20-120°C to give (R,S)-3-benzoylthio-2-Me propionyl chloride, then condensing with
 - (4S)-phenylthio-L-proline in the presence of base such as pyridine, KOH, etc. at pH = 5.0-12.0 and -20-120° to give
 - (4S)-[(2R)-benzoylthio-2-Me propionyl]-4-(phenylthio)-L-proline and (4S)-[(2S)-benzoylthio-2-Me propionyl]-4-(phenylthio)- L-proline; then
 - saltifing with amine such as aniline, cyclohexylamine, pyridine, etc. at mole ratio of 1:1.05-1.1; dissolving in acid solution, extracting with organic solvent(benzene, hexane, ether, Et acetate, etc.), and evaporating solvent to give (4S)-[(2R)-benzoylthio-2-Me propionyl]-4-(phenylthio)-L-proline. The
 - Zofenopril can be used for treating hypertension. Zofenopril synthesis acylation antihypertensive
- ST Zofenopri. IT Acvlation
 - Antihypertensives
 - (preparation of Zofenopril as antihypertensive)
- IT 7719-09-7, Thionyl chloride 7719-12-2, Trichlorophosphine 7791-25-5, Sulfonyl dichloride 10025-87-3, Phosphorus chloride oxide (PCl30) 10026-13-8, Phosphorus pentachloride
 - RL: RCT (Reactant); RACT (Reactant or reagent)
 - (as acylation agent)
- IT 110-86-1, Pyridine, uses 121-44-8, Triethylamine, uses 144-55-8, Sodium bicarbonate, uses 497-19-8, Sodium carbonate, uses 584-08-7, Potassium carbonate 1305-62-0, Calcium hydroxide, uses 1310-58-3, Potassium hydroxide, uses 1310-73-2, Sodium hydroxide, uses 7558-79-4, Sodium phosphate (Na2HPO4) 7601-54-9, Sodium phosphate (Ma3PO4) 7758-11-4, Potassium phosphate (K2HPO4) 7778-53-2, Potassium phosphate (K3PO4) 33752-731-8
 - RL: NUU (Other use, unclassified); USES (Uses)
 (as base for condensation reaction)
- IT 298-14-6, Potassium bicarbonate
 - RL: NUU (Other use, unclassified); USES (Uses) (as base for condensation reaction K2HPO4)
- IT 56-87-1, Lysine, uses 62-53-3, Aniline, uses 74-79-3, Arginine, uses 95-53-4, 2-Methylaniline, uses 101-83-7, Dicyclohexylamine 102-71-6,

uses 106-49-0, 4-Methylaniline, uses 107-15-3, 1,2-Diaminoethane, uses 108-01-0, N,N-Dimethylaminoethanol 108-91-8, Cyclohexylamine, 109-89-7, Diethylamine, uses 111-42-2, N,N-Diethanolamine, uses 122-39-4, Diphenvlamine, uses 1003-03-8, Cyclopentylamine 5452-35-7, Cvcloheptvlamine

RL: NUU (Other use, unclassified); USES (Uses)

(as organic base) 81872-10-8P, Zofenopril

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of Zofenopril as antihypertensive)

ΙT 74431-50-8 81653-77-2

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of Zofenopril as antihypertensive) 81938-38-7P 875303-98-3P 875303-99-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of Zofenopril as antihypertensive)

56-23-5, Carbon tetrachloride, uses 67-64-1, Acetone, uses 67-66-3, Chloroform, uses 67-68-5, DMSO, uses 68-12-2, DMF, uses 71-43-2, Benzene, uses 75-09-2, Methylene chloride, uses 78-93-3, Butanone, uses 108-88-3, Toluene, uses 109-99-9, THF, uses 123-91-1, Dioxane, uses 127-19-5, N,N-Dimethylacetamide 617-84-5, N,N-Diethylformamide 1300-21-6. Dichloroethane

RL: NUU (Other use, unclassified); USES (Uses) (solvent for acylation)

60-29-7, Diethyl ether, uses 64-17-5, Ethanol, uses 67-56-1, Methanol, uses 67-63-0, Isopropanol, uses 71-23-8, 1-Propanol, uses 71-36-3, 1-Butanol, uses 75-05-8, Acetonitrile, uses 78-83-1, Isobutanol, uses 79-20-9, Methyl acetate 107-21-1, 1,2-Ethanediol, uses 108-20-3, Diisopropyl ether 108-93-0, Cyclohexanol, uses 109-21-7, Butyl butanoate 123-51-3, Isopentanol 123-86-4, Butvl acetate 141-78-6, Ethyl acetate, uses 592-84-7, Butyl formate 1330-20-7, Xylene, uses 26264-14-2, Propanediol 525579-86-6, Hexanol RL: NUU (Other use, unclassified); USES (Uses)

(solvent for saltification)

L9 ANSWER 15 OF 55 CAPLUS COPYRIGHT 2009 ACS on STN

AN 2005:1280822 CAPLUS

144:162932 DN

ED Entered STN: 07 Dec 2005

ΤI Unexpected structural analogy between early and late 3d transition metal alkoxide carboxylates: Synthesis and single crystal X-ray study of Ni6(OH) 2(ORN) 6(OCOR) 2, RN = C2H4NMe2, R = H, CH3

AII Ilina, Elena; Kessler, Vadim G.

CS Department of Chemistry, Altay State University, Barnaul, Russia

SO Polyhedron (2005), 24(18), 3052-3056 CODEN: PLYHDE: ISSN: 0277-5387

- PB Elsevier B.V.
- DT Journal
- LA English
- CC 78-7 (Inorganic Chemicals and Reactions)

Section cross-reference(s): 75

- CASREACT 144:162932
- ΔR Modification of the liquid Ni(ORN)2, RN = C2H4NMe2, with stoichiometric or sub-stoichiometric amts. of carboxylic acids, HCOOH or CH3COOH, gave crystalline heteroleptic complexes Ni6(OH)2(ORN)6(OCOR)2, R = H (1), CH3 (3) with the core structure closely analogous to that observed earlier for hexanuclear Ti(IV) alkoxide carboxylates and derived from hexagonal packing of the donor atoms. The formate ligand in 1 could apparently be derived from oxidation of the amino alc. reactant by traces of

- oxygen, and the hydroxide ligands from water formed in the reaction.
- crystal structure nickel alkoxide carboxylate hydroxide hexanuclear cluster; nickel alkoxide carboxylate hydroxide hexanuclear cluster prepn structure
 - Crystal structure
 - Molecular structure
- (of hexanuclear nickel aminoethoxide carboxylate hydroxide clusters)
- Cluster compounds
 - RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (preparation and crystal structure of hexanuclear nickel aminoethoxide carboxylate hydroxide clusters)
 - 64-19-7, Acetic acid, 64-18-6, Formic acid, reactions
 - reactions 108-01-0, 2-(Dimethylamino)ethanol
 - 10534-88-0, Hexaamminenickel(2+) dichloride
 - RL: RCT (Reactant); RACT (Reactant or reagent)
 - (for preparation of hexanuclear nickel aminoethoxide carboxylate hydroxide cluster)
- 873778-74-6P 873778-78-0P
 - RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
- (preparation and crystal structure of)
- 873778-76-8P
 - RL: SPN (Synthetic preparation); PREP (Preparation)
- (preparation of) RE.CNT 19
- THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD
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- (19) Yang, E; Polyhedron 2003, V22, P1727 CAPLUS
- 1.9 ANSWER 16 OF 55 CAPLUS COPYRIGHT 2009 ACS on STN
- AN 2005:1168599 CAPLUS
- 144:88435 DN
- ED Entered STN: 03 Nov 2005
- Regioselective C-2 and C-6 Substitution of (S)-Nicotine and Nicotine
- Fevrier, Florence C.; Smith, Emilie D.; Comins, Daniel L.
- Department of Chemistry, North Carolina State University, Raleigh, NC, 27695-8204. USA
- SO Organic Letters (2005), 7(24), 5457-5460 CODEN: ORLEF7; ISSN: 1523-7060
- PB American Chemical Society
- Journal
- LA English
- 31-5 (Alkaloids)
- OS CASREACT 144:88435



Regioselective deprotonations of (S)-nicotine and derivs. I [R = H, SiMe3, SiMe2(CH2CH:CH2), SiMe2Ph] at the C-2 and C-6 positions of the pyridine ring were performed in good to excellent yields. These methodologies allow the direct introduction of a plethora of functional groups, e.g. iodo, chloro, and tributylstannyl, onto the pyridine ring of nicotine.

ST nicotine regioselective electrophilic substitution

IT Deprotonation

Substitution reaction, electrophilic

(regioselective; regioselective electrophilic substitution of (S)-nicotine and derivs.)

54-11-5, (S)-Nicotine 108-01-0, 2-(Dimethylamino) ethanol 109-94-4, Ethyl formate 852238-98-3

852619-88-6 872315-64-5

RL: RCT (Reactant); RACT (Reactant or reagent)

(regioselective electrophilic substitution of (S)-nicotine and derivs.) 75-77-4, Trimethylsilyl chloride, reactions 67-72-1, Hexachloroethane 128-08-5, N-Bromosuccinimide 594-82-1, Hexamethylethane 624-92-0, Dimethyldisulfide 768-33-2, Dimethylphenylsilyl chloride 1461-22-9, Chlorotributylstannane 3091-32-5, Chlorotricyclohexylstannane

7726-95-6, Bromine, reactions 16636-96-7, Di-tert-butyl zinc 29594-22-7

RL: RGT (Reagent); RACT (Reactant or reagent)

(regioselective electrophilic substitution of (S)-nicotine and derivs.) 96400-85-0P 112091-17-5P 853737-18-5P 40316-89-0P 80294-10-6P 853737-19-6P 853737-20-9P 853737-21-0P 853737-22-1P 872315-65-6P 872315-66-7P 872315-67-8P 872315-68-9P 872315-69-0P 872315-70-3P 872315-71-4P 872315-72-5P 872315-73-6P

RL: SPN (Synthetic preparation); PREP (Preparation)

(regioselective electrophilic substitution of (S)-nicotine and derivs.) RE.CNT 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD

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    ANSWER 17 OF 55 CAPLUS COPYRIGHT 2009 ACS on STN
AN
    2005:698085 CAPLUS
DN
    143:154240
ED
    Entered STN: 05 Aug 2005
TΙ
    Alkanolamines used as thermal stabilizers in production of homopolymers or
     copolymers of vinyl chloride with good thermal stability
IN
     Macho, Vendelin; Srokova, Iva; Beno, Lubos; Lucky, Martin; Gaman, Lubos;
    Mazanec, Jan; Cingelova, Jarmila; Hojc, Jan
PA
     Slovakia
SO
    Slovakia, 7 pp.
     CODEN: SLXXFO
     Patent
LA
     Slovak
     ICM C08F002-18
     ICS C08F002-22; C08F014-06
     37-3 (Plastics Manufacture and Processing)
FAN.CNT 1
    PATENT NO.
                        KIND DATE
                                           APPLICATION NO.
                                                                   DATE
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PI SK 284170 PRAI SK 2001-73 CLASS		B6 2004100 200101		20010115
PATENT NO.	CLASS	PATENT FAMILY	CLASSIFICATION CODES	
SK 284170	ICM ICS IPCI		BF014-06 CM,7]; C08F0002-22 [ICS,7], BF0014-06 [ICS,7]; C08F001-	
OS MARPAT 143:	154240			

AB

Vinyl chloride (co)polymers with good thermal stability are obtained by (co)polymerizing vinyl chloride, followed by addition of 0.01-1.2% (based on

the

polymer weight) of a water-soluble alkanolamine with the general formula RN(R')(R''), where R and R' are H, Me, Et, Pr, Bu, CnH2nOH and CnH2nOCnH2nOH, and R' is CnH2nOH and CnH2nOCnH2nOH, and n is 2-4, or a mixture of a water-soluble alkanolamine with a water-soluble salt of an alkali metal. Thus, a vinyl acetate-vinyl chloride copolymer was after preparation mixed with triethanolamine thermal stabilizer.

PVC thermal stabilization alkanolamine; vinyl chloride copolymer alkanolamine alkali metal salt thermal stabilizer

Heat stabilizers

(alkanolamines and optionally also alkali metal salts used as thermal stabilizers in production of thermally stable vinyl chloride (homo)polymers)

9002-86-2P, PVC 9003-22-9P, Vinyl acetate-vinyl chloride copolymer RL: IMF (Industrial manufacture); POF (Polymer in formulation); PREP (Preparation); USES (Uses)

(alkanolamines and optionally also alkali metal salts used as thermal stabilizers in production of thermally stable vinyl chloride

(homo)polymers)

- 102-71-6, Triethanolamine, uses 105-59-9, Methyldiethanolamine 108-01-0, Dimethylaminoethanol 111-42-2, Diethanolamine, uses 122-20-3, Triisopropanolamine 127-08-2, Potassium acetate 14 141-43-5, Monoethanolamine, uses 142-72-3, Magnesium acetate 497-19-8, Sodium carbonate, uses 557-39-1, Magnesium formate 7558-79-4, Disodium hydrogen phosphate 7631-99-4, Sodium nitrate, uses 7681-57-4. Sodium pyrosulfite 7757-79-1, Potassium nitrate, uses 70789-50-3 254448-29-8 860342-27-4 860342-28-5
 - RL: MOA (Modifier or additive use); USES (Uses)

(alkanolamines and optionally also alkali metal salts used as thermal stabilizers in production of thermally stable vinyl chloride (homo)polymers)

- 1.9 ANSWER 18 OF 55 CAPLUS COPYRIGHT 2009 ACS on STN
- AN 2005:71176 CAPLUS
- DN 142 • 176857
- ED Entered STN: 27 Jan 2005
- TΙ Preparation of fused anyl and heteroaryl derivatives, in particular pyrazolo[3,4-d]pyrimidines, as modulators of G-coupled protein receptor and their use in the prophylaxis and treatment of metabolic disorders
- IN Jones, Robert M.; Semple, Graeme; Xiong, Yifeng; Shin, Young-Jun; Ren, Albert S.; Calderon, Imelda; Fioravanti, Beatriz; Choi, Jin Sun Karoline; Sage, Carlton R.
- Arena Pharmaceuticals, Inc., USA
- PCT Int. Appl., 320 pp. SO
- CODEN: PIXXD2
- DT Patent
- LA English
- IC ICM C07D487-04
 - ICS C07D473-00; C07D498-04; C07D471-04; C07D215-22; A61K031-519; A61K031-52; A61K031-4375; A61K031-47; A61P003-00; A61P003-10
- 28-16 (Heterocyclic Compounds (More Than One Hetero Atom)) Section cross-reference(s): 1, 63

FAN.CNT 1

	PATENT NO.					KIND DATE			APPLICATION NO.										
PI		0 2005007658 0 2005007658							WO 2004-US22417										
		W:	AE,					AU, DE,											
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								LV,											
								PL.											
			TJ,	TM,	TN,	TR,	TT,	TZ,	UA,	UG,	US,	UZ,	VC,	VN,	YU,	ZA,	ZM,	ZW	
		RW:	BW,	GH,	GM,	KE,	LS,	MW,	ΜZ,	NA,	SD,	SL,	SZ,	TZ,	UG,	ZM,	ZW,	AM,	
								RU,											
								GR,											
						BF,	ВJ,	CF,	CG,	CI,	CM,	GA,	GN,	GQ,	GW,	ML,	MR,	NE,	
	2.11	2004		TD,		3.1		2005	0127		211.2	004	2572	c 7		2	0040	712	
										AU 2004-257267 CA 2004-2532971									
						A1 20050317													
						B2 20061107									20010123				
										EP 2004-756935					20040713				
		R:	AT,	BE,	CH,	DE,	DK,	ES,	FR,	GB,	GR,	IT,	LI,	LU,	NL,	SE,	MC,	PT,	
								RO,											HR
		1829						2006											
	BR	JP 2007531698			A		2006	1003		BR 2004-12689					2	0040	713		
											SG 2008-5436								
	ΤIA	IN Z006KN00071				A		2007	0/2/	IN 2006-KN71			20060109						

KR 20060569 MX 20060005 NO 20060006 US 20060142 US 20070072 US 20070082 PRAI US 2003-487 US 2004-890 WO 2004-052 CLASS PATENT NO.	54 88 262 844 874 443P 644P 549 2417	A 20060 A 20060 A 20060 A1 20060 A1 20070 A1 20070 P 20030 P 20031 A3 20040 W 20040 A1 20060 PATENT FAMILY	703 MX 407 NO 629 US 329 US 412 US 714 010 713 713 216	2006-700945 2006-554 2006-688 2006-355785 2006-602162 2006-602176	20060113 20060113 20060213 20060216 20061120 20061120						
WO 2005007658	ICM	C07D487-04									
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AU 2004257267	IPCI	[I,C]; A61K00 C07D0215-00 [[I,C]; C07D04 A61K0031-4375 [I,A]; A61K00 A61P0003-10 [[I,A]; C07D04	31-519 [I I,C]; C07 98-00 [I, [I,A]; A 31-52 [I, I,A]; C07 73-00 [I,	K0031-4353 [I,C]; A6 ,C]; A61P0003-00 [I, D0471-00 [I,C]; C07E C]; C07D0487-04 [I,A]; A6 61K0031-47 [I,A]; A6 A]; A61P0003-00 [I,A D0215-22 [I,A]; C07D0498-04 [I,A]	C]; 00473-00 1]; 51K0031-519 1]; 00471-04						
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CA 2532971	IPCI	A61K0031-4375 [I,A]; A61K00 A61P0003-00 [[I,A]; C07D02	[I,A]; A 31-519 [I I,A]; A61 15-00 [I,	C07D498/04+261B+239E 61K0031-4353 [1,C*]; ,A]; A61K0031-52 [1, P0003-10 [1,A]; C07D C*]; C07D0471-04 [1, 7D0473-00 [1,A]; C07	A61K0031-47 A]; 00215-22 A];						

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[I,A]; C07D0487-00 [I,C*]; C07D0498-04 [I,A];
                       C07D0498-00 [I,C*]
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                       C07D0487-00 [I,C]; C07D0487-04 [I,A]; A61K0031-4353
                       [I,C]; A61K0031-4375 [I,A]; A61K0031-47 [I,C];
                       A61K0031-47 [I,A]; A61K0031-519 [I,C]; A61K0031-519
                       [I,A]; A61K0031-52 [I,A]; A61P0003-00 [I,C];
                       A61P0003-00 [I,A]; A61P0003-10 [I,A]; C07D0215-00
                       [I,C]; C07D0215-22 [I,A]; C07D0215-233 [I,A];
                       C07D0471-00 [I,C]; C07D0471-04 [I,A]; C07D0473-00
                       [I,C]; C07D0473-00 [I,A]; C07D0498-00 [I,C];
                       C07D0498-04 [I.A]
                ECLA
                       C07D215/22C; C07D471/04+221B+221B+2;
                       C07D471/04+239B+221B; C07D473/00B2A;
                       C07D487/04+239B+231B; C07D487/04+239C+231C;
                       C07D487/04+249B+239B; C07D498/04+261B+239B
US 20050059650 TPCT
                       A61K0031-519 [I,A]; A61K0031-407 [I,A]; C07D0487-02
                       [I,A]; C07D0487-00 [I,C*]; C07D0471-12 [I,A];
                       C07D0471-00 [I,C*]
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                       C07D0215-00 [I,C*]; C07D0215-233 [I,A]; C07D0471-00
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                       C07D0473-00 [I,A]; C07D0487-00 [I,C*]; C07D0487-04
                       [I,A]; C07D0498-00 [I,C*]; C07D0498-04 [I,A];
                       A61K0031-519 [I,C]; A61K0031-519 [I,A]; A61K0031-407
                       [I,C]; A61K0031-407 [I,A]; C07D0215-22 [N,A];
                       C07D0471-12 [I,A]; C07D0487-02 [I,A]
                NCL.
                       514/210.210; 514/243.000; 514/248.000; 514/249.000;
                       514/259.410; 544/184.000; 544/236.000; 544/279.000;
                       544/350.000; 514/262.100; 514/303.000; 544/262.000;
                       546/119.000
                ECLA
                       C07D215/22C; C07D471/04+221B+221B+2;
                       C07D471/04+239B+221B; C07D473/00B2A;
                       C07D487/04+239B+231B; C07D487/04+239C+231C;
                       C07D487/04+249B+239B; C07D498/04+261B+239B; M07D
EP 1644375
                IPCI
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                       C07D0473-00 [ICS,7]; C07D0498-04 [ICS,7]; C07D0498-00
                       [ICS,7,C*]; C07D0471-04 [ICS,7]; C07D0471-00
                       [ICS,7,C*]; C07D0215-22 [ICS,7]; C07D0215-00
                       [ICS, 7, C*]; A61K0031-519 [ICS, 7]; A61K0031-52 [ICS, 7];
                       A61K0031-4375 [ICS, 7]; A61K0031-4353 [ICS, 7, C*];
                       A61K0031-47 [ICS, 7]; A61P0003-00 [ICS, 7]; A61P0003-10
                       [ICS, 7]
                IPCR
                       A61P0003-00 [I,C*]; A61P0003-00 [I,A]; A61P0003-10
                       [I,A]; C07D0215-00 [I,C*]; C07D0215-22 [N,A];
                       C07D0215-233 [I,A]; C07D0471-00 [I,C*]; C07D0471-04
                       [I,A]; C07D0473-00 [I,C*]; C07D0473-00 [I,A];
                       C07D0487-00 [I,C*]; C07D0487-04 [I,A]; C07D0498-00
                       [I,C*]; C07D0498-04 [I,A]
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                       C07D471/04+221B+221B+2; C07D473/00B2A;
                       C07D487/04+249B+239B; C07D487/04+239C+231C;
                       C07D487/04+239B+231B; C07D498/04+261B+239B; M07D
CN 1829718
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                       [I,A]; C07D0498-04 [I,A]; C07D0498-00 [I,C*];
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                       A61K0031-52 [I,A]; A61K0031-4375 [I,A]; A61K0031-4353
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                       A61P0003-10 [I,A]
BR 2004012689
                TPCT
                       C07D0487-04 [ICS,7]; C07D0487-00 [ICS,7,C*];
                       A61K0031-4375 [ICS,7]; A61K0031-4353 [ICS,7,C*];
                       A61K0031-47 [ICS, 7]; A61K0031-519 [ICS, 7]; A61K0031-52
                       [ICS, 7]; A61P0003-00 [ICS, 7]; A61P0003-10 [ICS, 7];
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C07D0215-22 [ICS,7]; C07D0215-00 [ICS,7,C*];
                       C07D0471-04 [ICS,7]; C07D0471-00 [ICS,7,C*];
                       C07D0473-00 [ICS, 7]; C07D0498-04 [ICS, 7]; C07D0498-00
                       [ICS, 7, C*]
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                       C07D471/04+221B+221B+2; C07D473/00B2A;
                       C07D487/04+249B+239B; C07D487/04+239C+231C;
                       C07D487/04+239B+231B; C07D498/04+261B+239B; M07D
JP 2007531698
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                       4C050/HH04; 4C063/AA01; 4C063/BB06; 4C063/CC14;
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                       4C072/GG07; 4C072/HH02; 4C072/HH07; 4C072/UU01;
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NO 2006000688
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                        C07D487/04+239B+231B; C07D498/04+261B+239B; M07D
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                        514/210.210; 514/262.100; 544/262.000
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US 20070072844
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                        C07D0471-04 [I,A]; C07D0473-00 [I,C*]; C07D0473-00
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                        C07D487/04+239B+231B; C07D498/04+261B+239B; M07D
US 20070082874 IPCI
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                        514/081.000; 514/262.100; 544/244.000; 544/262.000
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                        C07D471/04+221B+221B+2; C07D473/00B2A;
                        C07D487/04+249B+239B; C07D487/04+239C+231C;
                        C07D487/04+239B+231B; C07D498/04+261B+239B; M07D
    CASREACT 142:176857; MARPAT 142:176857
os
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^{*} STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Title compds. I [wherein A, B = independently (un)substituted alkylene; D = 0, S, SO, SO2, etc.; E = N, C, CH and derivs.; K = (un)substituted cyclo/alkylene; Q = NH and derivs., O, S, SO, SO2; T, M, J = independently

N, CH and derivs.; U, W, Z = independently C, N; V = a bond, N, CH and derivs.; X, Y = independently O, S, N, CH and derivs.; Arl = (un)substituted hetero/aryl; their pharmaceutically acceptable salts, hydrates and solvates] were prepared as modulators, in particular agonists and inverse agonists of G-coupled protein receptor (RUP3), for treating diabetes, hyperglycemia and other metabolic disorders. Ten biol. examples are given. For example, II was prepared, in 5 steps, from 4-(methylsulfonyl)phenylhydrazine=HCl, ethoxymethylenemalononitrile and 4-chloro-1-(4-methylsulfonylphenyl)-HH-pyrazolo[3, 4-d]pyrimidine. Selected I displayed BC50 < 10 µM in a melanophore-based pigment dispersion assay. Selected RUP3 agonists I lowered blood glucose levels in rats in an oral glucose tolerance test. Thus, I are useful in the prophylaxis or treatment of metabolic disorders and complications thereof, such as, diabetes and obesity.

ST pyrazolopyrimidine prepn metab G coupled protein receptor inverse agonist; diabetes obesity G coupled protein receptor agonist pyrazolopyrimidine prepn; hyperglycemia antidiabetic hypertriglyceridemia hypercholesterolemia fused aryl heteroaryl prepn

IT G protein-coupled receptors

RL: BSU (Biological study, unclassified); BIOL (Biological study) (agonists; preparation of fused aryl and heteroaryl derivs., in particular pyrazolopyrimidines, as modulators of G-coupled protein receptor and their use in treatment of diabetes, hyperglycemia and related diseases)

IT Autoimmune disease (insulin-dependent diabetes mellitus, treatment; preparation of fused aryl and heteroaryl derivs., in particular pyrazolopyrimidines, as modulators of G-coupled protein receptor and their use in treatment of diabetes, hyperolycemia and related diseases.

IT Diabetes mellitus

(insulin-dependent, treatment; preparation of fused aryl and heteroaryl derivs., in particular pyrazolopyrimidines, as modulators of G-coupled protein receptor and their use in treatment of diabetes, hyperglycemia and related diseases)

IT G protein-coupled receptors

RL. BSU (Biological study, unclassified); BIOL (Biological study) (inverse agonists; preparation of fused aryl and heteroaryl derivs., in particular pyrazolopyrimidines, as modulators of G-coupled protein receptor and their use in treatment of diabetes, hyperglycemia and related diseases)

IT Metabolic disorders

(metabolic syndrome X, treatment; preparation of fused aryl and heteroaryl derivs., in particular pyrazolopyrimidines, as modulators of G-coupled protein receptor and their use in treatment of diabetes, hyperglycemia and related diseases)

IT Diabetes mellitus

(non-insulin-dependent, treatment; preparation of fused aryl and heteroaryl dender, in particular pyrazolopyrimidines, as modulators of G-coupled protein receptor and their use in treatment of diabetes, hyperglycemia and related diseases.

IT Anticholesteremic agents

Antidiabetic agents

Human

Hypolipemic agents

(preparation of fused aryl and heteroaryl derivs., in particular pyrazolopyrimidines, as modulators of G-coupled protein receptor and their use in treatment of diabetes, hyperglycemia and related diseases)

IT Hypercholesterolemia

Hyperglycemia Hypertriglyceridemia Metabolic disorders Dyslipidemia Hyperlipidemia

```
RL: BIOL (Biological study)
   (treatment; preparation of fused anyl and heteroaryl derivs., in particular
   pyrazolopyrimidines, as modulators of G-coupled protein receptor and
   their use in treatment of diabetes, hyperglycemia and related diseases)
832714-06-4P, 4-[[1-(4-Methylsulfonylphenyl)-1H-pyrazolo[3,4-d]pyrimidin-4-
yl]oxy]piperidine-1-carboxylic acid tert-butyl ester 832714-19-9P,
1-(4-Methylsulfonylphenyl)-4-[(piperidin-4-yl)oxy]-1H-pyrazolo[3,4-
d]pyrimidine
             832714-42-8P, 1-(2-Fluoro-4-methylsulfonylphenyl)-4-
[(piperidin-4-vl)oxv]-1H-pvrazolo[3,4-d]pvrimidine 832714-45-1P,
4-[[1-(2-Fluoro-4-methylsulfonylphenyl)-1H-pyrazolo[3,4-d]pyrimidin-4-
yl]oxy]piperidine-1-carboxylic acid tert-butyl ester 832714-89-3P
832715-06-7P 832715-08-9P, 4-[[1-(2-Fluoro-4-methylsulfonylphenyl)-1H-
pyrazolo[3,4-d]pyrimidin-4-yl]sulfanyl]piperidine-1-carboxylic acid
tert-butyl ester 832715-45-4P, (5-Aminopyridin-2-y1)[4-[[1-(2-fluoro-4-
methylsulfonylphenyl)-1H-pyrazolo[3,4-d]pyrimidin-4-yl]oxy]piperidin-1-
yl]methanone trifluoroacetate 832715-50-1P,
4-[[1-(4-Bromophenyl)-1H-pyrazolo[3,4-d]pyrimidin-4-yl]oxy]piperidine-1-
carboxylic acid isopropyl ester 832715-72-7P,
trans-[4-[[1-(4-Methylsulfonylphenyl)-1H-pyrazolo[3,4-d]pyrimidin-4-
yl]amino|cyclohexyl|carbamic acid tert-butyl ester 832716-02-6P
832716-69-5P, 4-(1-Benzylazetidin-3-yloxy)-1-(4-methylsulfonylphenyl)-1H-
pyrazolo[3,4-d]pyrimidine 832717-22-3P,
4-[[3-(4-Methylsulfonylphenyl)isoxazolo[4,5-d]pyrimidin-7-
vlloxylpiperidine-1-carboxylic acid tert-butyl ester
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic
preparation); THU (Therapeutic use); BIOL (Biological study); PREP
(Preparation); RACT (Reactant or reagent); USES (Uses)
   (drug candidate; preparation of fused aryl and heteroaryl derivs., in
   particular pyrazolopyrimidines, as modulators of G-coupled protein
   receptor and their use in treatment of diabetes, hyperglycemia and
   related diseases)
352530-44-0P, 2-Fluoro-4-bromophenylzinc iodide
                                                832714-09-7P,
4-[[1-(4-Methylsulfonylphenyl)-3-methyl-1H-pyrazolo[3,4-d]pyrimidin-4-
                                                     832714-13-3P,
yl]oxy]piperidine-1-carboxylic acid tert-butyl ester
4-[[1-(4-Methylsulfonylphenyl)-3,6-dimethyl-1H-pyrazolo[3,4-d]pyrimidin-4-
yl]oxy]piperidine-1-carboxylic acid tert-butyl ester 832714-17-7P,
4-[[1-(4-Methylsulfonylphenyl)-1H-pyrazolo[3,4-d]pyrimidin-4-
yl]oxy]piperidine-1-carboxylic acid isobutyl ester 832714-18-8P,
4-[[1-(4-Methylsulfonylphenyl)-1H-pyrazolo[3,4-d]pyrimidin-4-
vl]oxy|piperidine-1-carboxylic acid isopropyl ester 832714-20-2P,
[4-[1-(4-Methylsulfonylphenyl)-1H-pyrazolo[3,4-d]pyrimidin-4-
vlloxylpiperidin-1-vllpyridin-3-ylmethanone 832714-21-3P.
4-[[1-(4-Methylsulfonylphenyl)-1H-pyrazolo[3,4-d]pyrimidin-4-
yl]oxy]piperidine-1-carboxylic acid butyl ester
                                                 832714-23-5P,
4-[[1-(2-Fluoro-4-methylsulfonylphenyl)-1H-pyrazolo[3,4-d]pyrimidin-4-
v1|sulfanv1|piperidine-1-carboxvlic acid cyclopropylmethyl ester
832714-25-7P, 4-[[1-(2-Fluoro-4-methylsulfonylphenyl)-1H-pyrazolo[3,4-
d]pyrimidin-4-yl]sulfanyl]piperidine-1-carboxylic acid cyclobutylmethyl
ester 832714-26-8P, 4-[[1-(2-Fluoro-4-methylsulfonylphenyl)-1H-
pyrazolo[3, 4-d]pyrimidin-4-yl]sulfanyl]piperidine-1-carboxylic acid
2-cyclopropylethyl ester 832714-27-9P,
(5-Bromofuran-2-yl)[4-[[1-(2-fluoro-4-methylsulfonylphenyl)-1H-
pvrazolo[3, 4-d]pvrimidin-4-v1|sulfanvl|piperidin-1-v1|methanone
832714-28-0P, 4-[[1-(4-Methylsulfonylphenyl)-1H-pyrazolo[3,4-d]pyrimidin-4-
yl]oxy]piperidine-1-carboxylic acid pentyl ester 832714-29-1P,
4-[[1-(4-Methylsulfonylphenyl)-1H-pyrazolo[3,4-d]pyrimidin-4-
yl]oxy]piperidine-1-carboxylic acid 1-ethylpropyl ester
                                                         832714-30-4P,
4-[[1-(4-Methylsulfonylphenyl)-1H-pyrazolo[3,4-d]pyrimidin-4-
yl]oxy]piperidine-1-carboxylic acid 2-ethylbutyl ester
                                                         832714-31-5P,
4-[[1-(4-Methylsulfonylphenyl)-1H-pyrazolo[3,4-d]pyrimidin-4-
yl]oxy]piperidine-1-carboxylic acid cyclopentylmethyl ester
```

832714-32-6P, 4-[[1-(4-Methylsulfonylphenyl)-1H-pyrazolo[3,4-d]pyrimidin-4-

```
vl]oxy]piperidine-1-carboxylic acid 2,2-dimethylpropyl ester
832714-33-7P, (5-Butylpyridin-2-y1)[4-[[1-(4-methylsulfonylphenyl)-1H-
pyrazolo[3,4-d]pyrimidin-4-y1]oxy]piperidin-1-y1]methanone
                                                            832714-34-8P,
(4-Difluoromethoxyphenyl)[4-[[1-(2-fluoro-4-methylsulfonylphenyl)-1H-
pyrazolo[3,4-d]pyrimidin-4-yl]oxy]piperidin-1-yl]methanone
                                                           832714-36-0P.
1-(2-Fluoro-4-methylsulfonylphenyl)-4-[[1-(3-isopropyl-[1,2,4]oxadiazol-5-
vl)piperidin-4-vl]oxy]-1H-pyrazolo[3,4-d]pyrimidine 832714-40-6P,
2-[4-[1-(2-Fluoro-4-methylsulfonylphenyl)-1H-pyrazolo[3,4-d]pyrimidin-4-
v1|oxv|piperidin-1-v1|-1-(4-trifluoromethoxyphenv1)ethanone
832714-43-9P, 2-[4-[[1-(2-Fluoro-4-methylsulfonylphenyl])-1H-pyrazolo[3,4-
d|pyrimidin-4-v||oxy|piperidin-1-v||-1-(3-fluorophenyl)ethanone
832714-44-0P, 2-[4-[[1-(2-Fluoro-4-methylsulfonylphenyl)-1H-pyrazolo[3,4-
d]pyrimidin-4-yl]oxy]piperidin-1-yl]-1-(pyridin-2-yl)ethanone
832714-46-2P, 4-||1-(2-Fluoro-4-methylsulfonylphenyl)-1H-pyrazolo|3,4-
d]pyrimidin-4-yl]oxy]piperidine-1-carboxylic acid isopropyl ester
832714-50-8P, (4-Ethylpyridin-2-yl)[4-[[1-(2-fluoro-4-
methylsulfonylphenyl)-1H-pyrazolo[3,4-d]pyrimidin-4-yl]oxy]piperidin-1-
vllmethanone
              832714-51-9P, (5-Bromopyridin-3-yl)[4-[[1-(2-fluoro-4-
methylsulfonylphenyl)-1H-pyrazolo[3,4-d]pyrimidin-4-yl]oxy]piperidin-1-
              832714-52-0P, (5-Ethylpyridin-2-yl)[4-[[1-(2-fluoro-4-
vl]methanone
methylsulfonylphenyl)-1H-pyrazolo[3,4-d]pyrimidin-4-yl]oxy|piperidin-1-
vllmethanone
              832714-53-1P, (4-Ethoxyphenyl)[4-[[1-(2-fluoro-4-
methylsulfonylphenyl)-1H-pyrazolo[3,4-d]pyrimidin-4-yl[0xy]piperidin-1-
vllmethanone
              832714-54-2P, (5-Butylpyridin-2-v1)[4-[[1-(2-fluoro-4-
methylsulfonylphenyl)-1H-pyrazolo[3,4-d]pyrimidin-4-yl]oxy]piperidin-1-
              832714-55-3P, [4-[[1-(2-Fluoro-4-methylsulfonylphenyl)-1H-
vllmethanone
pyrazolo[3,4-d]pyrimidin-4-vl]oxy[piperidin-1-vl](5-
isopropoxymethylpyridin-2-yl)methanone 832714-59-7P,
[4-[(1-(2-Fluoro-4-methylsulfonylphenyl)-1H-pyrazolo(3,4-d)pyrimidin-4-
vlloxylpiperidin-1-vll(5-isopropoxypyridin-2-vl)methanone 832714-61-1P.
4-[[1-(2-Fluoro-4-methylsulfonylphenyl)-1H-pyrazolo[3,4-d]pyrimidin-4-
yl]oxy]-5'-isopropoxy-3,4,5,6-tetrahydro-2H-[1,2']bipyridinyl
832714-63-3P, 1-(2-Fluoro-4-methylsulfonylphenyl)-4-[[1-(4-
trifluoromethoxyphenyl)piperidin-4-yl]oxy]-1H-pyrazolo[3,4-d]pyrimidine
832714-64-4P, 1-(2-Fluoro-4-methylsulfonylphenyl)-4-[[1-(3-
trifluoromethoxyphenyl)piperidin-4-yl]oxy]-1H-pyrazolo[3,4-d]pyrimidine
832714-65-5P, 5'-Fluoro-4-[[1-(4-methylsulfonylphenyl)-1H-pyrazolo[3,4-
d]pyrimidin-4-yl]oxy]-3,4,5,6-tetrahydro-2H-[1,2']bipyridinyl
832714-66-6P, 4-[[1-(4-Methylsulfonylphenyl)-1H-pyrazolo[3,4-d]pyrimidin-4-
v1]oxv]-5'-methv1-3,4,5,6-tetrahydro-2H-[1,2']bipyridinv1 832714-67-7P,
4-[[1-(4-Methylsulfonvlphenyl)-1H-pyrazolo[3,4-d]pyrimidin-4-yl]oxyl-6'-
trifluoromethyl-3, 4, 5, 6-tetrahydro-2H-[1, 2']bipyridinyl
                                                         832714-68-8P.
(5'-Fluoro-3, 4, 5, 6-tetrahydro-2H-[1,2']bipyridinvl-4-vl) [1-(4-
methylsulfonylphenyl)-1H-pyrazolo[3,4-d]pyrimidin-4-yl]amine
832714-69-9P, (6-Chloropyridin-3-yl)[4-[[1-(4-methylsulfonylphenyl)-1H-
pyrazolo[3,4-d]pyrimidin-4-vl]oxy[piperidin-1-yl]methanone 832714-70-2P,
(5-Chloropyridin-3-vl)[4-[[1-(4-methylsulfonylphenyl)-1H-pyrazolo[3,4-
d|pvrimidin-4-vl|oxv|piperidin-1-vl|methanone
                                              832714-71-3P,
[4-[1-(4-Methylsulfonylphenyl)-1H-pyrazolo[3,4-d]pyrimidin-4-
yl]oxy]piperidin-1-yl](1-methyl-3-trifluoromethyl-1H-pyrazol-4-
               832714-72-4P, (2-Chloropyridin-4-yl)[4-[[1-(4-
yl)methanone
methylsulfonylphenyl)-1H-pyrazolo[3,4-d]pyrimidin-4-yl]oxy|piperidin-1-
vllmethanone
              832714-74-6P, (4-Hvdroxv-3-methoxyphenvl)[4-[[1-(4-
methylsulfonylphenyl)-1H-pyrazolo[3,4-d]pyrimidin-4-yl]oxy]piperidin-1-
vllmethanone
              832714-75-7P, (4-Chloro-3-nitrophenyl)[4-[[1-(4-
methylsulfonvlphenyl)-1H-pyrazolo[3,4-d]pyrimidin-4-yl]oxy]piperidin-1-
vllmethanone
              832714-76-8P, 1-[4-[[1-(4-Methylsulfonylphenyl)-1H-
pyrazolo[3,4-d]pyrimidin-4-yl]oxy]piperidin-1-yl]-3-methylbutan-1-one
832714-77-9P, [4-[[1-(4-Methylsulfonylphenyl)-1H-pyrazolo[3,4-d]pyrimidin-
4-yl]oxy]piperidin-1-yl][6-(pyrazol-1-yl)pyridin-3-yl]methanone
832714-78-0P, (2-Hydroxypyridin-3-y1)[4-[[1-(4-methylsulfonylphenyl)-1H-
pyrazolo[3,4-d]pyrimidin-4-yl]oxy]piperidin-1-yl]methanone 832714-79-1P,
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(5,6-Dichloropyridin-3-yl)[4-[[1-(4-methylsulfonylphenyl)-1H-pyrazolo[3,4-
d|pyrimidin-4-v1|oxy|piperidin-1-v1|methanone
                                               832714-80-4P,
(5-Bromopyridin-3-y1)[4-[[1-(4-methylsulfonylphenyl)-1H-pyrazolo[3,4-
d]pyrimidin-4-yl]oxy]piperidin-1-yl]methanone
                                               832714-81-5P,
5-[[4-[[1-(4-Methylsulfonylphenyl)-1H-pyrazolo[3,4-d]pyrimidin-4-
yl]oxy]piperidin-1-yl]carbonyl]nicotinic acid
                                                832714-82-6P.
(1H-Imidazol-4-yl)[4-[[1-(4-methylsulfonylphenyl)-1H-pyrazolo[3,4-
d]pyrimidin-4-y1]oxy]piperidin-1-y1]methanone 832714-83-7P,
[4-[[1-(4-Methylsulfonvlphenyl)-1H-pyrazolo[3,4-d]pyrimidin-4-
vlloxylpiperidin-1-vll[6-(pyrrolidin-1-vl)pyridin-3-vl]methanone
832714-84-8P, (6-Isobutylaminopyridin-3-v1)[4-[[1-(4-methylsulfonylphenyl)-
1H-pyrazolo[3,4-d]pyrimidin-4-y1]oxy]piperidin-1-y1]methanone
832714-85-9P, (6-Ethylaminopyridin-3-yl)[4-[[1-(4-methylsulfonylphenyl)-1H-
pyrazolo[3, 4-d]pyrimidin-4-yl]oxy]piperidin-1-yl]methanone
                                                           832714-86-0P,
[6-(Cyclobutylamino)pyridin-3-yl][4-[[1-(4-methylsulfonylphenyl)-1H-
pyrazolo[3, 4-d]pyrimidin-4-yl]oxy]piperidin-1-yl]methanone
                                                           832714-87-1P,
(6-Isopropylaminopyridin-3-yl)[4-[[1-(4-methylsulfonylphenyl)-1H-
pyrazolo[3,4-d]pyrimidin-4-yl]oxy]piperidin-1-yl]methanone
                                                           832714-88-2P.
[6-(1-Ethylpropylamino)pyridin-3-yl][4-[[1-(4-methylsulfonylphenyl)-1H-
pyrazolo[3,4-d]pyrimidin-4-yl]oxy]piperidin-1-yl]methanone
                                                            832714-91-7P.
[4-[[1-(4-Methylsulfonylphenyl)-1H-pyrazolo[3,4-d]pyrimidin-4-
v1]oxy[piperidin-1-v1][6-(1-propylbutvlamino)pyridin-3-v1]methanone
832714-93-9P
              832714-94-0P, (Benzo[c]isoxazol-3-v1)[4-[[1-(4-
methylsulfonylphenyl)-1H-pyrazolo[3,4-d]pyrimidin-4-ylloxylpiperidin-1-
               832714-96-2P, (4-Chloropyridin-2-v1)[4-[[1-(4-
vllmethanone
methylsulfonylphenyl)-1H-pyrazolo[3,4-d]pyrimidin-4-yl]oxy]piperidin-1-
              832714-98-4P, 1-[4-[[1-(4-Methylsulfonylphenyl)-1H-
vllmethanone
pyrazolo[3,4-d]pyrimidin-4-v1]oxy[piperidin-1-v1]butan-2-one
832715-00-1P
              832715-01-2P, 5'-Bromo-4-[[1-(4-methylsulfonylphenyl)-1H-
pyrazolo[3,4-d]pyrimidin-4-yl]oxy]-3,4,5,6-tetrahydro-2H-[1,2']bipyridinyl
832715-02-3P, 4-[[1-(4-Methylsulfonylphenyl)-1H-pyrazolo[3,4-d]pyrimidin-4-
yl]oxy]-5'-trifluoromethyl-3,4,5,6-tetrahydro-2H-[1,2']bipyridinyl
832715-04-5P, 1-[2-Fluoro-4-(methylsulfonyl)phenyl]-4-[[1-(3-isopropyl-
1,2,4-oxadiazol-5-yl)-3-pyrrolidinyl]oxy]-1H-pyrazolo[3,4-d]pyrimidine
              832715-07-8P, 1-[4-(Methylsulfonyl)phenyl]-4-[[1-[4-
hvdrochloride
(trifluoromethoxy)phenyl]-4-piperidinyl]oxy]-1H-pyrazolo[3,4-d]pyrimidine
hydrochloride
              832715-09-0P, 4-[[1-(2-Fluoro-4-methylsulfonylphenyl)-1H-
pyrazolo[3,4-d]pyrimidin-4-yl]sulfanyl]piperidine-1-carboxylic acid
isopropyl ester
                 832715-10-3P, [4-[[1-(4-Methylsulfonylphenyl)-1H-
pyrazolo[3,4-d]pyrimidin-4-yl]oxy]piperidin-1-yl](5-methylpyridin-3-
vl)methanone
              832715-11-4P,
[4-[[1-(4-Methylsulfonylphenyl)-1H-pyrazolo[3,4-d]pyrimidin-4-
vlloxy|piperidin-1-vl|(5-methy|pyridin-3-vl)methanone trifluoroacetate
832715-12-5P, [4-[[1-(4-Methylsulfonylphenyl)-1H-pyrazolo[3,4-d]pyrimidin-
4-yl]oxy]piperidin-1-yl](6-trifluoromethylpyridin-3-yl)methanone
832715-13-6P, [4-[[1-(4-Methylsulfonylphenyl)-1H-pyrazolo[3,4-d]pyrimidin-
4-v1]oxy|piperidin-1-v1](6-trifluoromethylpyridin-3-v1)methanone
                 832715-14-7P, 2-(5-Bromopyridin-3-yl)-1-[4-[[1-(4-
trifluoroacetate
methylsulfonylphenyl)-1H-pyrazolo[3,4-d]pyrimidin-4-yl]oxy]piperidin-1-
              832715-15-8P, 2-(5-Bromopyridin-3-yl)-1-[4-[[1-(4-
vllethanone
methylsulfonylphenyl)-1H-pyrazolo[3,4-d]pyrimidin-4-yl]oxy]piperidin-1-
vl]ethanone trifluoroacetate
                              832715-16-9P,
(6-Fluoropyridin-2-v1)[4-[[1-(4-methylsulfonylphenyl)-1H-pyrazolo[3,4-
d|pvrimidin-4-vl|oxv|piperidin-1-vl|methanone
                                              832715-17-0P.
(6-Fluoropyridin-2-yl)[4-[[1-(4-methylsulfonylphenyl)-1H-pyrazolo[3,4-
d]pyrimidin-4-yl]oxy]piperidin-1-yl]methanone trifluoroacetate
832715-18-1P, (6-Chloropyridin-2-yl)[4-[[1-(4-methylsulfonvlphenyl)-1H-
pyrazolo[3, 4-d]pyrimidin-4-yl]oxy]piperidin-1-yl]methanone
                                                            832715-19-2P.
(6-Chloropyridin-2-yl)[4-[[1-(4-methylsulfonylphenyl)-1H-pyrazolo[3,4-
d]pyrimidin-4-yl]oxy]piperidin-1-yl]methanone trifluoroacetate
832715-20-5P, [4-[[1-(4-Methylsulfonylphenyl)-1H-pyrazolo[3,4-d]pyrimidin-
4-yl]oxy]piperidin-1-yl][5-[(2-methylpyrrolidin-1-yl)methyl]pyridin-3-
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vllmethanone
               832715-21-6P, [4-[[1-(4-Methylsulfonylphenyl)-1H-
pyrazolo[3,4-d]pyrimidin-4-yl]oxy[piperidin-1-yl][5-[(2-methylpyrrolidin-1-
v1)methv1|pvridin-3-v1|methanone trifluoroacetate
                                                  832715-22-7P,
5-[[4-[[1-(4-Methylsulfonylphenyl)-1H-pyrazolo[3,4-d]pyrimidin-4-
vlloxylpiperidin-1-yllcarbonyllnicotinonitrile 832715-23-8P.
5-[[4-[[1-(4-Methylsulfonylphenyl)-1H-pyrazolo[3,4-d]pyrimidin-4-
yl]oxy]piperidin-1-yl]carbonyl]nicotinonitrile trifluoroacetate
832715-24-9P, 5-[[4-[[1-(4-Methylsulfonylphenyl)-1H-pyrazolo[3,4-
d|pvrimidin-4-vl|oxv|piperidin-1-vl|carbonvl|pvridine-2-carboxvlic acid
methyl ester 832715-25-0P, 5-[[4-[[1-(4-Methylsulfonylphenyl)-1H-
pyrazolo[3,4-d]pyrimidin-4-yl]oxy]piperidin-1-yl]carbonyl]pyridine-2-
carboxylic acid methyl ester trifluoroacetate 832715-26-1P.
[4-[[1-(4-Methylsulfonylphenyl)-1H-pyrazolo[3,4-d]pyrimidin-4-
yl]oxy]piperidin-1-yl]acetic acid ethyl ester 832715-27-2P,
[4-[[1-(4-Methylsulfonylphenyl)-1H-pyrazolo[3,4-d]pyrimidin-4-
yl]oxy]piperidin-1-yl]acetic acid ethyl ester trifluoroacetate
832715-28-3P, 1-(4-Chlorophenyl)-2-[4-[[1-(4-methylsulfonylphenyl)-1H-
pyrazolo[3,4-d]pyrimidin-4-yl]oxy]piperidin-1-yl]ethanone 832715-29-4P,
 -(4-Chlorophenyl)-2-[4-[[1-(4-methylsulfonylphenyl)-1H-pyrazolo[3,4-
d]pyrimidin-4-yl]oxy]piperidin-1-yl]ethanone trifluoroacetate
832715-30-7P, 2-[4-[[1-(4-Methylsulfonylphenyl)-1H-pyrazolo[3,4-
d|pvrimidin-4-v1|oxv|piperidin-1-v1|-1-(3-trifluoromethylphenyl)ethanone
832715-31-8P, 2-[4-[[1-(4-Methylsulfonylphenyl)-1H-pyrazolo[3,4-
d|pvrimidin-4-v1|oxv|piperidin-1-v1|-1-(3-trifluoromethylphenyl)ethanone
trifluoroacetate 832715-32-9P, 1-(4-Chloro-3-methylphenyl)-2-[4-[[1-(4-
methylsulfonylphenyl)-1H-pyrazolo[3,4-d]pyrimidin-4-yl]oxy]piperidin-1-
            832715-33-0P, 1-(4-Chloro-3-methylphenyl)-2-[4-[[1-(4-
vl]ethanone
methylsulfonylphenyl)-1H-pyrazolo[3,4-d]pyrimidin-4-ylloxy|piperidin-1-
vllethanone trifluoroacetate 832715-34-1P,
1-(3,4-Dichlorophenyl)-2-[4-[[1-(4-methylsulfonylphenyl)-1H-pyrazolo[3,4-
d]pyrimidin-4-yl]oxy]piperidin-1-yl]ethanone 832715-35-2P,
1-(3,4-Dichlorophenyl)-2-[4-[[1-(4-methylsulfonylphenyl)-1H-pyrazolo[3,4-
d]pyrimidin-4-vl]oxy]piperidin-1-vl]ethanone trifluoroacetate
832715-36-3P, 1-(2,4-Dimethoxyphenyl)-2-[4-[[1-(4-methylsulfonylphenyl)-1H-
pyrazolo[3,4-d]pyrimidin-4-yl]oxy]piperidin-1-yl]ethanone 832715-37-4P,
1-(2,4-Dimethoxyphenyl)-2-[4-[[1-(4-methylsulfonylphenyl)-1H-pyrazolo[3,4-
d]pyrimidin-4-yl]oxy]piperidin-1-yl]ethanone trifluoroacetate
832715-38-5P, 1-(4-Difluoromethoxyphenyl)-2-[4-[[1-(4-
methylsulfonylphenyl)-1H-pyrazolo[3,4-d]pyrimidin-4-yl]oxy]piperidin-1-
             832715-39-6P, 1-(4-Difluoromethoxyphenyl)-2-[4-[[1-(4-
vl]ethanone
methylsulfonylphenyl)-1H-pyrazolo[3,4-d]pyrimidin-4-yl]oxy]piperidin-1-
vllethanone trifluoroacetate 832715-40-9P,
1-(4-Diethylaminophenyl)-2-[4-[[1-(4-methylsulfonylphenyl)-1H-pyrazolo[3,4-
d]pyrimidin-4-yl]oxy]piperidin-1-yl]ethanone 832715-41-0P,
1-(4-Diethylaminophenyl)-2-[4-[[1-(4-methylsulfonylphenyl)-1H-pyrazolo[3,4-
d]pvrimidin-4-vl]oxv]piperidin-1-vl]ethanone trifluoroacetate
832715-42-1P, (5-Aminopyridin-2-v1)[4-[[1-(4-methylsulfonylphenyl)-1H-
pyrazolo[3,4-d]pyrimidin-4-ylloxylpiperidin-1-yllmethanone
(5-Aminopyridin-2-yl)[4-[[1-(4-methylsulfonylphenyl)-1H-pyrazolo[3,4-
d]pyrimidin-4-yl]oxy]piperidin-1-yl]methanone trifluoroacetate
832715-44-3P, (5-Aminopyridin-2-yl)[4-[[1-(2-fluoro-4-
methylsulfonylphenyl)-1H-pyrazolo[3,4-d]pyrimidin-4-yl]oxy]piperidin-1-
v1]methanone
              832715-46-5P,
(5-Ethylaminopyridin-2-vl)[4-[[1-(2-fluoro-4-methylsulfonylphenyl)-1H-
pyrazolo[3,4-d]pyrimidin-4-yl]oxy]piperidin-1-yl]methanone
(5-Ethylaminopyridin-2-yl)[4-[[1-(2-fluoro-4-methylsulfonylphenyl)-1H-
pyrazolo[3,4-d]pyrimidin-4-yl]oxy]piperidin-1-yl]methanone
trifluoroacetate
                  832715-48-7P, [4-[[1-(2-Fluoro-4-methylsulfonylphenyl)-
1H-pyrazolo[3,4-d]pyrimidin-4-yl]oxy]piperidin-1-yl][5-(3-
methylbutylamino)pyridin-2-yl]methanone 832715-49-8P,
[4-[[1-(2-Fluoro-4-methylsulfonylphenyl)-1H-pyrazolo[3,4-d]pyrimidin-4-
yl]oxy]piperidin-1-yl][5-(3-methylbutylamino)pyridin-2-yl]methanone
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trifluoroacetate
                  832715-53-4P, 4-[[1-(4-Propylaminophenyl)-1H-
pyrazolo[3,4-d]pyrimidin-4-vl[oxy]piperidine-1-carboxylic acid isopropyl
       832715-54-5P, 4-[[1-(4-Isopropylaminophenyl)-1H-pyrazolo[3,4-
d|pvrimidin-4-vl|oxv|piperidine-1-carboxvlic acid isopropvl ester
832715-55-6P, 4-[[1-[4-(Morpholin-4-y1)pheny1]-1H-pyrazolo[3,4-d]pyrimidin-
4-yl]oxy]piperidine-1-carboxylic acid isopropyl ester 832715-56-7P,
4-[[1-(2-Fluoro-4-isopropylaminophenyl)-1H-pyrazolo[3,4-d]pyrimidin-4-
yl]oxy[piperidine-1-carboxylic acid isopropyl ester 832715-58-9P,
4-[[1-[2-Fluoro-4-(morpholin-4-v1)phenv1]-1H-pvrazolo[3,4-d]pvrimidin-4-
vlloxy/piperidine-1-carboxylic acid isopropyl ester 832715-59-0P.
4-[[1-[4-[4-(2-Methylsulfonylethyl)piperazin-1-yl]-2-methylphenyl]-1H-
pyrazolo[3,4-d]pyrimidin-4-yl]oxy]piperidine-1-carboxylic acid isopropyl
ester 832715-61-4P, 4-[[1-[2-Methyl-4-[(tetrahydrofuran-2-
vlmethyl)amino|phenyl|-1H-pyrazolo[3,4-d|pyrimidin-4-yl]oxy|piperidine-1-
carboxylic acid isopropyl ester 832715-62-5P,
4-[[1-(4-Cyclopropylamino-2-methylphenyl)-1H-pyrazolo[3,4-d]pyrimidin-4-
yl]oxy]piperidine-1-carboxylic acid isopropyl ester 832715-63-6P,
4-[[1-[4-(2-Dimethylaminoethylamino)-2-methylphenyl]-1H-pyrazolo[3,4-
d]pyrimidin-4-yl]oxy]piperidine-1-carboxylic acid isopropyl ester
832715-64-7P, 4-[[1-[4-[(2-Methylsulfonylethyl)(methyl)amino]phenyl]-1H-
pyrazolo[3,4-d]pyrimidin-4-vl]oxy|piperidine-1-carboxylic acid isopropyl
      832715-65-8P, 4-[[1-[4-(2-Methoxyethylamino)phenyl]-1H-
pyrazolo[3,4-d]pyrimidin-4-vl]oxy|piperidine-1-carboxylic acid isopropyl
      832715-66-9P, 4-[[1-[4-[(Tetrahydrofuran-2-vlmethyl)amino]phenyl]-
1H-pyrazolo[3,4-d]pyrimidin-4-yl]oxy]piperidine-1-carboxylic acid
                832715-67-0P, 4-[[1-[4-[4-(2-
isopropyl ester
Methylsulfonylethyl)piperazin-1-yl|phenyl|-1H-pyrazolo[3,4-d]pyrimidin-4-
yl]oxy]piperidine-1-carboxylic acid isopropyl ester 832715-68-1P,
4-[[1-(4-Aminophenyl)-1H-pyrazolo[3,4-d]pyrimidin-4-yl]oxy]piperidine-1-
carboxylic acid isopropyl ester
                                832715-69-2P.
4-[1-(5-Ethylpyrimidin-2-yl)piperidin-4-ylsulfanyl]-1-(2-fluoro-4-
methylsulfonylphenyl)-1H-pyrazolo[3,4-d]pyrimidine 832715-70-5P,
3-tert-Butoxy-1-[4-[[1-(4-methylsulfonylphenyl)-1H-pyrazolo[3,4-
d]pyrimidin-4-yl]oxy]piperidin-1-yl]propan-1-one 832715-71-6P,
[3-[4-[[1-(4-Methylsulfonylphenyl)-1H-pyrazolo[3,4-d]pyrimidin-4-
yl]oxy]piperidin-1-yl]-3-oxopropyl](methyl)carbamic acid tert-butyl ester
832715-73-8P, trans-N-[1-(4-Methylsulfonylphenyl)-1H-pyrazolo[3,4-
d]pyrimidin-4-yl]cyclohexane-1,4-diamine 832715-74-9P,
cis-N-[4-[[1-(4-Methylsulfonylphenyl)-1H-pyrazolo[3,4-d]pyrimidin-4-
vl]amino|cvclohexvl|nicotinamide
                                 832715-75-0P
                                                 832715-76-1P,
cis-[4-[[[1-(4-Methylsulfonylphenyl)-1H-pyrazolo[3,4-d]pyrimidin-4-
vllamino|methyl|cyclohexyl|carbamic acid tert-butyl ester 832715-77-2P.
cis-N-[[4-[[1-(4-Methylsulfonylphenyl)-1H-pyrazolo[3,4-d]pyrimidin-4-
yl]amino]cyclohexyl]methyl]nicotinamide 832715-78-3P,
cis-N-[[4-[[1-(4-Methylsulfonylphenyl)-1H-pyrazolo[3,4-d]pyrimidin-4-
v1]amino|cvclohexv1|methv1|-6-methv1nicotinamide 832715-79-4P,
4-[2-[Ethyl][1-(4-methylsulfonylphenyl)-1H-pyrazolo[3,4-d]pyrimidin-4-
vllaminolethyllpiperazine-1-carboxylic acid tert-butyl ester
832715-80-7P, 4-[[[1-(2-Fluoro-4-methylsulfonylphenyl)-1H-pyrazolo[3,4-
d]pyrimidin-4-yl]isopropylamino]methyl]piperidine-1-carboxylic acid
tert-butyl ester 832715-81-8P, 4-[[[1-(2-Fluoro-4-methylsulfonylphenyl)-
1H-pyrazolo[3,4-d]pyrimidin-4-yl]isopropylamino[methyl]piperidine-1-
carboxylic acid isopropyl ester
                                832715-82-9P,
4-[[1-(2-Fluoro-4-sulfamoylphenyl)-1H-pyrazolo[3,4-d]pyrimidin-4-
yl]oxy]piperidine-1-carboxylic acid isopropyl ester 832715-83-0P,
(1-tert-Buty1-5-methy1-1H-pyrazo1-4-y1)[4-[[1-(4-methy1sulfony1pheny1)-1H-
pyrazolo[3,4-d]pyrimidin-4-yl]oxy]piperidin-1-yl]methanone 832715-84-1P,
(5-tert-Butyl-2-methyl-2H-pyrazol-3-yl)[4-[[1-(4-methylsulfonylphenyl)-1H-
pyrazolo[3,4-d]pyrimidin-4-yl]oxy]piperidin-1-yl]methanone 832715-85-2P,
(3-Fluorophenyl)[4-[[1-(4-methylsulfonylphenyl)-1H-pyrazolo[3,4-
d]pyrimidin-4-y1]oxy]piperidin-1-y1]methanone 832715-87-4P,
1-(2-Fluoro-4-methylsulfonylphenyl)-4-[[1-[(3-isopropyl-[1,2,4]oxadiazol-5-
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yl)methyl]piperidin-4-yl]oxy]-1H-pyrazolo[3,4-d]pyrimidine
                                                                832715-88-5P
, 4-[[1-(4-Methylsulfonylphenyl)-1H-pyrazolo[3,4-d]pyrimidin-4-
                                                           832715-90-9P.
    vl]amino|piperidine-1-carboxvlic acid isopropyl ester
     4-[[1-(4-Methylsulfonylphenyl)-1H-pyrazolo[3,4-d]pyrimidin-4-
    vllaminolpiperidine-1-carboxylic acid isobutyl ester 832715-91-0P.
    [3-[[1-(4-Methylsulfonylphenyl)-1H-pyrazolo[3,4-d]pyrimidin-4-
    yl]amino]piperidin-1-yl](6-methylpyridin-3-yl)methanone
                                                             832715-93-2P.
    [3-[1-(4-Methylsulfonylphenyl)-1H-pyrazolo[3,4-d]pyrimidin-4-
    vllaminolpiperidin-1-vll(2-methylpyridin-3-vl)methanone 832715-94-3P,
    [3-[1-(4-Methylsulfonylphenyl)-1H-pyrazolo[3,4-d]pyrimidin-4-
    yl]amino]piperidin-1-yl](5-methylpyridin-3-yl)methanone 832715-95-4P,
    [3-[1-(4-Methylsulfonylphenyl)-1H-pyrazolo[3,4-d]pyrimidin-4-
    yl]amino]piperidin-1-yl]pyridin-3-ylmethanone 832715-96-5P,
     [3-[1-(4-Methylsulfonylphenyl)-1H-pyrazolo[3,4-d]pyrimidin-4-
    yl]amino]piperidin-1-yl](1-methyl-1H-pyrrol-3-yl)methanone 832715-97-6P,
    [4-[[1-(4-Methylsulfonylphenyl)-1H-pyrazolo[3,4-d]pyrimidin-4-
    yl]oxy]piperidin-1-yl](4-trifluoromethylpyridin-3-yl)methanone
    832715-98-7P, (6-tert-Butylpyridin-3-yl)[4-[[1-(4-methylsulfonylphenyl)-1H-
    pyrazolo[3,4-d]pyrimidin-4-yl]oxy]piperidin-1-yl]methanone 832716-00-4P,
     4-[[[1-(4-Methylsulfonylphenyl)-1H-pyrazolo[3,4-d]pyrimidin-4-
    vl]amino]methyl]piperidine-1-carboxylic acid tert-butyl ester
    832716-01-5P, 4-[[[1-(4-Methylsulfonylphenyl)-1H-pyrazolo[3,4-d]pyrimidin-
     4-vll(methyl)aminolmethyllpiperidine-1-carboxylic acid tert-butyl ester
    832716-03-7P, 3-[[[1-(4-Methylsulfonylphenyl)-1H-pyrazolo[3,4-d]pyrimidin-
     4-yl]amino]methyl]piperidine-1-carboxylic acid tert-butyl ester
    832716-04-8P, 4-[[Ethyl[1-(4-methylsulfonylphenyl)-1H-pyrazolo[3,4-
    d]pyrimidin-4-yl]amino]methyl]piperidine-1-carboxylic acid tert-butyl
            832716-05-9P, 4-[[1-[2-(2-Dimethylaminoethoxy)-4-
    methylsulfonylphenyl]-1H-pyrazolo[3,4-d]pyrimidin-4-yl]oxy]piperidine-1-
    carboxylic acid tert-butyl ester 832716-08-2P,
    4-[[(2-Dimethylaminoethyl)][1-(4-methylsulfonylphenyl)-1H-pyrazolo[3,4-
    d]pyrimidin-4-yl]amino]methyl]piperidine-1-carboxylic acid tert-butyl
            832716-11-7P, 4-[[(2-Dimethylaminoethyl)]1-(2-fluoro-4-
    methylsulfonylphenyl)-1H-pyrazolo[3,4-d]pyrimidin-4-
    vllamino|methvl|piperidine-1-carboxvlic acid tert-butvl ester
    832716-13-9P, [4-[[1-(2-Fluoro-4-methylsulfonylphenyl)-1H-pyrazolo[3,4-
    d|pvrimidin-4-v1|oxy|piperidin-1-y1](4-trifluoromethoxypheny1)methanone
    832716-15-1P, [4-[[1-[3,5-Bis(trifluoromethyl)phenyl]-1H-pyrazolo[3,4-
    d]pyrimidin-4-yl]amino]cyclohexyl]carbamic acid tert-butyl ester
    832716-17-3P, 4-[[1-[3,5-Bis(trifluoromethyl)phenyl]-1H-pyrazolo[3,4-
    dlpvrimidin-4-vlloxylpiperidine-1-carboxylic acid tert-butyl ester
    832716-19-5P
                   832716-21-9P, 4-[[1-(3-Fluorophenyl)-1H-pyrazolo[3,4-
    dlpvrimidin-4-vlloxylpiperidine-1-carboxylic acid tert-butyl ester
    832716-23-1P, [4-[[1-(3-Fluorophenyl)-1H-pyrazolo[3,4-d]pyrimidin-4-
    yl]amino]cyclohexyl]carbamic acid tert-butyl ester
                                                         832716-25-3P.
    cis-[4-[[1-(2,4-Difluorophenyl)-1H-pyrazolo[3,4-d]pyrimidin-4-
    vl]amino]cvclohexvl]carbamic acid tert-butvl ester
                                                         832716-26-4P,
    4-[[1-(2,4-Difluorophenyl)-1H-pyrazolo[3,4-d]pyrimidin-4-yl]oxylpiperidine-
    1-carboxvlic acid tert-butyl ester 832716-28-6P,
    trans-[4-[[1-(4-Methylsulfonylphenyl)-1H-pyrazolo[3,4-d]pyrimidin-4-
    yl]oxy]cyclohexyl]carbamic acid tert-butyl ester
                                                       832716-30-0P,
    N-[1-(2,4-Difluorophenyl)-1H-pyrazolo[3,4-d]pyrimidin-4-yl]cyclohexane-1,4-
              832716-32-2P, 4-[[1-(2,5-Difluorophenv1)-1H-pvrazolo[3,4-
    d]pyrimidin-4-yl]oxy]piperidine-1-carboxylic acid tert-butyl ester
    832716-33-3P, 4-[[[1-[4-(2-Methylsulfonylethyl)phenyl]-1H-pyrazolo[3,4-
    d]pyrimidin-4-yl] (methyl) amino]methyl]piperidine-1-carboxylic acid
    tert-butyl ester
                       832716-35-5P, 4-[[[1-(2,5-Difluorophenyl)-1H-
    pyrazolo[3, 4-d]pyrimidin-4-yl] (methyl) amino] methyl]piperidine-1-carboxylic
    acid tert-butyl ester
                            832716-36-6P,
    4-[[1-(2-Methyl-4-propylaminophenyl)-1H-pyrazolo[3,4-d]pyrimidin-4-
    yl]oxy]piperidine-1-carboxylic acid isopropyl ester 832716-37-7P,
    4-[[1-(4-Isopropylamino-2-methylphenyl)-1H-pyrazolo[3,4-d]pyrimidin-4-
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yl]oxy]piperidine-1-carboxylic acid isopropyl ester
                                                      832716-38-8P.
4-[[1-[2-Methyl-4-(morpholin-4-yl)phenyl]-1H-pyrazolo[3,4-d]pyrimidin-4-
yl]oxy]piperidine-1-carboxylic acid isopropyl ester 832716-39-9P,
4-[[1-[4-(2-Methoxyethylamino)-2-methylphenyl]-1H-pyrazolo[3,4-d]pyrimidin-
4-yl]oxy]piperidine-1-carboxylic acid isopropyl ester 832716-41-3P,
4-[[1-[4-[(2-Methylsulfonylethyl)(methyl)amino]-2-methylphenyl]-1H-
pyrazolo[3,4-d]pyrimidin-4-yl]oxy]piperidine-1-carboxylic acid isopropyl
       832716-42-4P, [2-[4-[]1-(2-Fluoro-4-methylsulfonylphenyl)-1H-
pyrazolo[3,4-d]pyrimidin-4-v1]oxy[piperidin-1-v1]-5-methylpyrimidin-4-
vlldimethylamine 832716-46-8P, Furan-2-vl[4-[[1-(4-methylsulfonylphenyl)-
1H-pyrazolo[3,4-d]pyrimidin-4-yl]oxy]piperidin-1-yl]methanone
832716-47-9P, [4-[[1-(4-Methylsulfonylphenyl)-1H-pyrazolo[3,4-d]pyrimidin-
4-y1]oxy]piperidin-1-y1](1-methy1-1H-pyrro1-2-y1)methanone 832716-48-0P,
2-[4-[[1-(4-Methylsulfonylphenyl)-1H-pyrazolo[3,4-d]pyrimidin-4-
yl]oxy[piperidin-1-yl]-1-(pyridin-3-yl)ethanone 832716-49-1P,
2-[4-[[1-(4-Methylsulfonylphenyl)-1H-pyrazolo[3,4-d]pyrimidin-4-
yl]oxy]piperidin-1-yl]-1-(thiophen-2-yl)ethanone 832716-50-4P,
1-[4-[[1-(4-Methylsulfonylphenyl)-1H-pyrazolo[3,4-d]pyrimidin-4-
yl]oxy]piperidin-1-yl]-3,3-dimethylbutan-2-one 832716-51-5P,
[4-[[1-(4-Methylsulfonylphenyl)pyrazolo[3,4-d]pyrimidin-4-yl]oxy]piperidin-
1-v1|(2-methylpyridin-3-v1)methanone 832716-52-6P,
[4-[1-(4-Methylsulfonvlphenyl)-1H-pyrazolo[3,4-d]pyrimidin-4-
vlloxy|piperidin-1-vl|(6-methylpyridin-3-vl)methanone 832716-53-7P,
[4-[1-(4-Methylsulfonylphenyl)-1H-pyrazolo[3,4-d]pyrimidin-4-
yl]oxy]piperidin-1-yl](5-methylisoxazol-3-yl)methanone
                                                       832716-54-8P.
4-[[6-Dimethylamino-1-(4-methylsulfonylphenyl)-1H-pyrazolo[3,4-d]pyrimidin-
4-yl]oxy[piperidine-1-carboxylic acid tert-butyl ester 832716-57-1P,
4-[[Ethyl[1-(2-fluoro-4-methylsulfonylphenyl]-1H-pyrazolo[3,4-d]pyrimidin-
4-vllamino|methyl|piperidine-1-carboxylic acid isopropyl ester
832716-58-2P, 4-[[1-(2-Dimethylamino-4-methylsulfonylphenyl)-1H-
pyrazolo[3,4-d]pyrimidin-4-yl]oxy]piperidine-1-carboxylic acid tert-butyl
       832716-60-6P, 4-[2-[[1-(4-Methylsulfonylphenyl)-1H-pyrazolo[3,4-
d]pyrimidin-4-yl|oxy|ethyl|piperazine-1-carboxylic acid ethyl ester
832716-61-7P, 4-[2-[[1-(4-Methylsulfonylphenyl)-1H-pyrazolo[3,4-
d]pyrimidin-4-yl]oxy|propyl]piperazine-1-carboxylic acid ethyl ester
832716-62-8P, (5-Fluoropyridin-2-yl)[4-[[1-(4-methylsulfonylphenyl)-1H-
pyrazolo[3,4-d]pyrimidin-4-yl]oxy]piperidin-1-yl]methanone
(2-Chloro-5-fluoropyridin-3-yl)[4-[[1-(4-methylsulfonylphenyl)-1H-
pyrazolo[3,4-d]pyrimidin-4-yl]oxy]piperidin-1-yl]methanone
[4-[[1-(4-Methylsulfonylphenyl)-1H-pyrazolo[3,4-d]pyrimidin-4-
vlloxylpiperidin-1-vll(4-methoxypyridin-2-vl)methanone
                                                       832716-65-1P,
(2-Fluoropyridin-3-yl)[4-[[1-(4-methylsulfonylphenyl)-1H-pyrazolo[3,4-
d]pyrimidin-4-yl]oxy]piperidin-1-yl]methanone
                                               832716-66-2P.
(6-Fluoropyridin-3-yl)[4-[[1-(4-methylsulfonylphenyl)-1H-pyrazolo[3,4-
d]pyrimidin-4-yl]oxy]piperidin-1-yl]methanone
                                              832716-67-3P,
(4-Iodopyridin-2-v1)[4-[[1-(4-methylsulfonylphenyl)-1H-pyrazolo[3,4-
d]pvrimidin-4-v1]oxv[piperidin-1-v1]methanone 832716-68-4P,
[4-[(1-(4-Methylsulfonylphenyl)-1H-pyrazolo[3,4-d]pyrimidin-4-
yl]oxy]piperidin-1-yl](4-methoxythiophen-3-yl)methanone
                                                         832716-70-8P.
3-[[1-(4-Methylsulfonylphenyl)-1H-pyrazolo[3,4-d]pyrimidin-4-
yl]oxy]azetidine-1-carboxylic acid isopropyl ester
                                                    832716-72-0P,
[4-[1-(2-Fluoro-4-methylsulfonylphenyl)-1H-pyrazolo[3,4-d]pyrimidin-4-
vl]oxv[piperidin-1-vl](3-trifluoromethoxyphenvl)methanone
                                                           832716-73-1P,
4-[[1-(4-Methylsulfonylphenyl)-1H-pyrazolo[3,4-d]pyrimidin-4-
yl]oxy]piperidine-1-carboxylic acid propyl ester 832716-74-2P,
4-[[1-(4-Methylsulfonylphenyl)-1H-pyrazolo[3,4-d]pyrimidin-4-
yl]oxy]piperidine-1-carboxylic acid cyclohexyl ester
                                                       832716-75-3P.
4-[[1-(4-Methylsulfonylphenyl)-1H-pyrazolo[3,4-d]pyrimidin-4-
yl]oxy]piperidine-1-carboxylic acid tetrahydropyran-4-yl ester
832716-76-4P, 4-[[1-(4-Methylsulfonylphenyl)-1H-pyrazolo[3,4-d]pyrimidin-4-
yl]oxy]piperidine-1-carboxylic acid cyclopentyl ester 832716-78-6P,
4-[[1-(4-Methylsulfonylphenyl)-1H-pyrazolo[3,4-d]pyrimidin-4-
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yl]oxy]piperidine-1-carboxylic acid tetrahydrothiopyran-4-yl ester
832716-79-7P, 4-[[1-(4-Methylsulfonylphenyl)-1H-pyrazolo[3,4-d]pyrimidin-4-
vl]oxv[piperidine-1-carboxvlic acid cvclobutvl ester
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
(Uses)
   (drug candidate; preparation of fused aryl and heteroaryl derivs., in
   particular pyrazolopyrimidines, as modulators of G-coupled protein
   receptor and their use in treatment of diabetes, hyperglycemia and
   related diseases)
832716-80-0P, 4-[[1-(4-Methylsulfonylphenyl)-1H-pyrazolo[3,4-d]pyrimidin-4-
yl]oxy]piperidine-1-carboxylic acid pyridin-3-ylmethyl ester
832716-81-1P, 4-[[1-(4-Methylsulfonylphenyl)-1H-pyrazolo[3,4-d]pyrimidin-4-
vl]oxy|piperidine-1-carboxylic acid 2-(pyridin-3-yl)ethyl ester
832716-82-2P, 4-[[1-(4-Methylsulfonylphenyl)-1H-pyrazolo[3,4-d]pyrimidin-4-
yl]oxy]piperidine-1-carboxylic acid 3-(pyridin-3-yl)propyl ester
832716-83-3P, 4-[[1-(4-Methylsulfonylphenyl)-1H-pyrazolo[3,4-d]pyrimidin-4-
yl]oxy]piperidine-1-carboxylic acid 2-dimethylaminoethyl ester
832716-84-4P, 4-[[1-(4-Methylsulfonylphenyl)-1H-pyrazolo[3,4-d]pyrimidin-4-
yl] (methyl) amino]piperidine-1-carboxylic acid tert-butyl ester
832716-85-5P, 1-[4-[[1-(4-Methylsulfonvlphenyl)-1H-pyrazolo[3,4-
d]pyrimidin-4-yl](methyl)amino]piperidin-1-yl]-3,3-dimethylbutan-2-one
832716-86-6P, 4-[[1-(4-Methylsulfonylphenyl)-1H-pyrazolo[3,4-d]pyrimidin-4-
vll(methyl)amino|piperidine-1-carboxylic acid cyclobutyl ester
832716-87-7P, 4-[[1-(4-Methylsulfonylphenyl)-1H-pyrazolo[3,4-d]pyrimidin-4-
vl]sulfanyl|piperidine-1-carboxylic acid tert-butyl ester
                                                           832716-88-8P.
4-[[1-(4-Methylsulfonvlphenvl)-1H-pyrazolo[3,4-d]pyrimidin-4-
vl|sulfinvl|piperidine-1-carboxvlic acid tert-butvl ester
                                                           832716-89-9P,
4-[[1-(4-Methylsulfonylphenyl)-1H-pyrazolo[3,4-d]pyrimidin-4-
yl]sulfonyl]piperidine-1-carboxylic acid tert-butyl ester 832716-90-2P,
4-[[1-(2-Fluoro-4-methylsulfonylphenyl)-1H-pyrazolo[3,4-d]pyrimidin-4-
yl]sulfanyl]piperidine-1-carboxylic acid butyl ester 832716-92-4P,
4-[[1-(2-Fluoro-4-methylsulfonylphenyl)-1H-pyrazolo[3,4-d]pyrimidin-4-
yl]sulfanyl]piperidine-1-carboxylic acid 2-methoxyethyl ester
832716-93-5P, 4-[[1-(2-Fluoro-4-methylsulfonylphenyl)-1H-pyrazolo[3,4-
d]pyrimidin-4-yl]sulfanyl]piperidine-1-carboxylic acid 3,3-dimethylbutyl
       832716-94-6P, 4-[[1-(2-Fluoro-4-methylsulfonylphenyl)-1H-
pyrazolo[3,4-d]pyrimidin-4-yl]sulfanyl]piperidine-1-carboxylic acid
4-methylpentyl ester
                      832716-95-7P,
[4-[1-(4-Methylsulfonylphenyl)-1H-pyrazolo[3,4-d]pyrimidin-4-
vlloxv|piperidin-1-vl|[5-[(morpholin-4-vl)methvl]furan-2-vl]methanone
832716-96-8P, 4-[[1-(4-Methylsulfonylphenyl)-1H-pyrazolo[3,4-d]pyrimidin-4-
vl]oxv|piperidine-1-carboxylic acid 2-(pyrrolidin-1-yl)ethyl ester
832716-97-9P, 4-[[1-(4-Methylsulfonylphenyl)-1H-pyrazolo[3,4-d]pyrimidin-4-
yl]oxy]piperidine-1-carboxylic acid 2-(morpholin-4-yl)ethyl ester
832716-98-0P, 4-[[1-(4-Methylsulfonylphenyl)-1H-pyrazolo[3,4-d]pyrimidin-4-
vl]oxv|piperidine-1-carboxvlic acid ethyl ester
                                                 832716-99-1P,
Ethyl[1-(2-fluoro-4-methylsulfonylphenyl)-1H-pyrazolo[3,4-d]pyrimidin-4-
yl][(3,4,5,6-tetrahydro-2H-[1,2']bipyridinyl-4-yl)methyl]amine
832717-01-8P, Ethyl[1-(2-fluoro-4-methylsulfonylphenyl)-1H-pyrazolo[3,4-
d]pyrimidin-4-yl][(5'-trifluoromethyl-3,4,5,6-tetrahydro-2H-
[1,2']bipyridinyl-4-yl)methyl]amine
                                    832717-02-9P
                                                    832717-05-2P,
3-[[1-(2-Fluoro-4-methylsulfonylphenyl)-1H-pyrazolo[3,4-d]pyrimidin-4-
yl]oxy]pyrrolidine-1-carboxylic acid tert-butyl ester 832717-06-3P,
3-[[1-(4-Methylsulfonylphenyl)-1H-pyrazolo[3,4-d]pyrimidin-4-
yl]amino]pyrrolidine-1-carboxylic acid tert-butyl ester 832717-07-4P.
3-[[1-(2-Fluoro-4-methylsulfonylphenyl)-1H-pyrazolo[3,4-d]pyrimidin-4-
yl]amino]pyrrolidine-1-carboxylic acid isopropyl ester 832717-09-6P,
3-[[1-(4-Methylsulfonylphenyl)-1H-pyrazolo[3,4-d]pyrimidin-4-
yl]oxy]pyrrolidine-1-carboxylic acid tert-butyl ester
                                                       832717-10-9P,
[4-[[1-(4-Methylsulfonylphenyl)-1H-pyrazolo[3,4-d]pyrimidin-4-
yl]oxy]piperidin-1-yl][5-(pyridin-2-yl)thiophen-2-yl]methanone
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832717-11-0P, 4-[[9-(6-Methylsulfonylpyridin-3-yl)-9H-purin-6-
vl]oxy|piperidine-1-carboxylic acid isobutyl ester 832717-12-1P,
9-(6-Methylsulfonylpyridin-3-yl)-6-[(piperidin-4-yl)oxy]-9H-purine
832717-13-2P, [4-[[9-(6-Methylsulfonylpyridin-3-y1)-9H-purin-6-
vlloxylpiperidin-1-vllpyridin-3-vlmethanone 832717-14-3P.
4-[[9-(4-Methylsulfonylphenyl)-9H-purin-6-yl]oxy]piperidine-1-carboxylic
acid tert-butyl ester 832717-17-6P,
4-[[9-(6-Methylsulfonylpyridin-3-yl)-9H-purin-6-yl]oxy[piperidine-1-
carboxvlic acid tert-butvl ester 832717-19-8P,
4-[[9-(2-Fluoro-4-methylsulfonvlphenvl)-9H-purin-6-vlloxylpiperidine-1-
carboxylic acid tert-butyl ester 832717-20-1P,
4-[[3-(4-Methylsulfonylphenyl)-3H-[1,2,3]triazolo[4,5-d]pyrimidin-7-
yl]oxy]piperidine-1-carboxylic acid tert-butyl ester 832717-30-3P,
4-[[Ethyl]3-(4-methylsulfonylphenyl)isoxazolo[4,5-d]pyrimidin-7-
yl]amino]methyl]piperidine-1-carboxylic acid tert-butyl ester
832717-31-4P, 4-[[3-(4-Methylsulfonylphenyl)isoxazolo[4,5-d]pyrimidin-7-
yl]sulfanyl]piperidine-1-carboxylic acid tert-butyl ester 832717-32-5P,
4-[[3-(4-Methylsulfonylphenyl)isoxazolo[4,5-d]pyrimidin-7-
yl]oxy]piperidine-1-carboxylic acid isopropyl ester
                                                    832717-33-6P,
4-[8-(4-Bromo-2-fluorophenyl)quinolin-4-yloxy|piperidine-1-carboxylic acid
isopropyl ester 832717-37-0P, 4-[[8-(4-Methylsulfanylphenyl)quinolin-4-
vlloxylpiperidine-1-carboxylic acid isopropyl ester 832717-39-2P.
4-[8-(4-Methylsulfonylphenyl)quinolin-4-yl]oxylpiperidine-1-carboxylic
acid isopropyl ester
                     832717-40-5P.
4-[8-(4-Isopropoxyphenyl)quinolin-4-yloxy]piperidine-1-carboxylic acid
                832717-41-6P, 2-[4-[[1-(4-Methylsulfonylphenyl)-1H-
isopropyl ester
pyrazolo[3,4-d]pyrimidin-4-yl]oxy[piperidin-1-yl]-1-(pyridin-2-yl)ethanone
832717-42-7P, [4-[[1-(4-Methylsulfonvlphenvl)-1H-pyrazolo[3,4-d]pyrimidin-
4-y1]oxy]piperidin-1-y1]pyrazin-2-ylmethanone 832717-43-8P,
[4-[[1-(4-Methylsulfonylphenyl)-1H-pyrazolo[3,4-d]pyrimidin-4-
yl]oxy]piperidin-1-yl](5-methylpyrazin-2-yl)methanone 832717-44-9P,
[4-[[1-(4-Methylsulfonylphenyl)-1H-pyrazolo[3,4-d]pyrimidin-4-
vl]oxy|piperidin-1-vl|pvrimidin-5-vlmethanone 832717-45-0P,
[4-[[1-(4-Methylsulfonylphenyl)-1H-pyrazolo[3,4-d]pyrimidin-4-
yl]oxy]piperidin-1-yl]pyridazin-4-ylmethanone 832717-46-1P,
[4-[[1-(4-Methylsulfonylphenyl)-1H-pyrazolo[3,4-d]pyrimidin-4-
yl]oxy]piperidin-1-yl]thiophen-2-ylmethanone
                                             832717-47-2P.
(3,4-Dimethylisoxazol-5-yl)[4-[[1-(4-methylsulfonylphenyl)-1H-pyrazolo[3,4-
d]pyrimidin-4-yl]oxy]piperidin-1-yl]methanone
                                              832717-48-3P,
[4-[1-(4-Methylsulfonvlphenyl)-1H-pyrazolo[3,4-d]pyrimidin-4-
vlloxvlpiperidin-1-vll(4-methyl-[1,2,3]thiadiazol-5-vl)methanone
832717-49-4P, (2,5-Dimethyl-2H-pyrazol-3-yl)[4-[[1-(4-
methylsulfonylphenyl)-1H-pyrazolo[3,4-d]pyrimidin-4-yl]oxy|piperidin-1-
             832717-50-7P, [4-[[1-(4-Methylsulfonylphenyl)-1H-
yl]methanone
pyrazolo[3,4-d]pyrimidin-4-yl]oxy[piperidin-1-yl](3-methylisoxazol-5-
vl)methanone
             832717-51-8P, 4-[[1-(4-Methylsulfonylphenyl)-1H-
pvrazolo[3,4-d]pvrimidin-4-v1]oxv[piperidine-1-carbothioic acid
N-(pvridin-4-vl)amide
                      832717-52-9P.
3-[[1-(2-Fluoro-4-methylsulfonylphenyl)-1H-pyrazolo[3,4-d]pyrimidin-4-
yl]amino]piperidine-1-carboxylic acid tert-butyl ester 832717-53-0P,
(2,5-Dimethylfuran-3-yl)[4-[[1-(4-methylsulfonylphenyl)-1H-pyrazolo[3,4-
d]pyrimidin-4-yl]oxy]piperidin-1-yl]methanone
                                               832717-54-1P,
1-(2-Fluoro-4-methylsulfonylphenyl)-4-[[1-[(3-isopropyl-[1,2,4]oxadiazol-5-
yl)methyl]pyrrolidin-3-yl]oxy]-1H-pyrazolo[3,4-d]pyrimidine
832717-55-2P, [4-[[1-(4-Methylsulfonylphenyl)-1H-pyrazolo[3,4-d]pyrimidin-
4-y1]oxy]piperidin-1-y1](6-methylpyridin-2-y1)methanone 832717-56-3P,
(2-Fluoropyridin-4-yl) [4-[[1-(4-methylsulfonylphenyl)-1H-pyrazolo[3,4-
d]pyrimidin-4-y1]oxy]piperidin-1-y1]methanone 832717-57-4P,
1-(4-Methylsulfonylphenyl)-4-[[1-(4-trifluoromethoxyphenyl)piperidin-4-
yl]oxy]-1H-pyrazolo[3,4-d]pyrimidine 832717-58-5P,
1-(2-Fluoro-4-methylsulfonylphenyl)-4-[[1-[5-methyl-4-(pyrrolidin-1-
yl)pyrimidin-2-yl]piperidin-4-yl]oxy]-1H-pyrazolo[3,4-d]pyrimidine
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832717-59-6P, 4-[[1-(2-Fluoro-4-propionylsulfamoylphenyl)-1H-pyrazolo[3,4-
d|pyrimidin-4-y1|oxy|piperidine-1-carboxylic acid isopropyl ester
832717-60-9P, 4-[[1-(4-Cyano-2-fluorophenyl)-1H-pyrazolo[3,4-d]pyrimidin-4-
vlloxy|piperidine-1-carboxylic acid isopropyl ester
                                                     832717-61-0P,
1-(2,5-Difluoro-4-methoxyphenyl)-4-[4-(3-isopropyl-[1,2,4]oxadiazol-5-
yl)cyclohexyloxy]-1H-pyrazolo[3,4-d]pyrimidine 832717-62-1P,
4-[[1-(2,5-Difluoro-4-methylsulfonylphenyl)-1H-pyrazolo[3,4-d]pyrimidin-4-
vl]oxy]piperidine-1-carboxylic acid isopropyl ester
                                                      832717-63-2P,
4-[[1-(4-Fluoro-6-methoxypyridin-3-vl)-1H-pyrazolo[3,4-d]pyrimidin-4-
vlloxylpiperidine-1-carboxylic acid isopropyl ester 832717-64-3P.
4-[[1-(6-Methoxy-2-methylpyridin-3-yl)-1H-pyrazolo[3,4-d]pyrimidin-4-
yl]oxy]piperidine-1-carboxylic acid isopropyl ester 832717-65-4P.
4-[[1-(2,5-Difluoro-4-sulfamoylphenyl)-1H-pyrazolo[3,4-d]pyrimidin-4-
vl]oxy|piperidine-1-carboxylic acid isopropyl ester 832717-66-5P,
4-[[1-(2-Fluoro-4-hydroxyphenyl)-1H-pyrazolo[3,4-d]pyrimidin-4-
yl]oxy]piperidine-1-carboxylic acid isopropyl ester 832717-67-6P,
3-Fluoro-4-[4-[[1-(3-isopropyl-[1,2,4]oxadiazol-5-yl)piperidin-4-
yl]oxy]pyrazolo[3,4-d]pyrimidin-1-yl]-N-propionylbenzenesulfonamide
832717-68-7P, 3-Fluoro-4-[4-[[1-(3-isopropyl-[1,2,4]oxadiazol-5-
vl)piperidin-4-vl]oxy]pyrazolo[3,4-d]pyrimidin-1-vl]benzonitrile
832717-69-8P, 3-Fluoro-4-[4-[[1-(3-isopropyl-[1,2,4]oxadiazol-5-
v1)piperidin-4-v1]oxv|pvrazolo[3,4-d]pvrimidin-1-v1]benzenesulfonamide
832717-70-1P, 1-(2,5-Difluoro-4-methylsulfonylphenyl)-4-[[1-(3-isopropyl-
[1,2,4]oxadiazol-5-vl)piperidin-4-vl]oxv]-1H-pyrazolo[3,4-d]pyrimidine
832717-71-2P, 1-(4-Fluoro-6-methoxypyridin-3-yl)-4-[[1-(3-isopropyl-
[1,2,4]oxadiazol-5-yl)piperidin-4-yl]oxy]-1H-pyrazolo[3,4-d]pyrimidine
832717-72-3P, 4-[[1-(3-Isopropyl-[1,2,4]oxadiazol-5-yl)piperidin-4-yl]oxy]-
1-(6-methoxy-2-methylpyridin-3-yl)-1H-pyrazolo[3,4-d]pyrimidine
832717-73-4P, 2,5-Difluoro-4-[4-[[1-(3-isopropyl-[1,2,4]oxadiazol-5-
yl)piperidin-4-yl]oxy]pyrazolo[3,4-d]pyrimidin-1-yl]benzenesulfonamide
832717-74-5P, 1-(2-Fluoro-4-methylsulfonylphenyl)-4-[4-(3-isopropyl-
[1,2,4]oxadiazol-5-yl)cyclohexyloxy]-1H-pyrazolo[3,4-d]pyrimidine
832717-75-6P, 3-Fluoro-4-[4-[4-(3-isopropyl-[1,2,4]oxadiazol-5-
v1)cvclohexvloxv|pvrazolo[3,4-d]pvrimidin-1-v1]-N-
propionylbenzenesulfonamide 832717-76-7P,
3-Fluoro-4-[4-[4-(3-isopropyl-[1,2,4]oxadiazol-5-
yl)cyclohexyloxy]pyrazolo[3,4-d]pyrimidin-1-vl]benzonitrile
832717-77-8P, 3-Fluoro-4-[4-[4-(3-isopropyl-[1,2,4]oxadiazol-5-
yl)cyclohexyloxy]pyrazolo[3,4-d]pyrimidin-1-yl]benzenesulfonamide
832717-78-9P, 1-(2,5-Difluoro-4-methylsulfonylphenyl)-4-[4-(3-isopropyl-
[1,2,4]oxadiazol-5-vl)cvclohexvloxvl-1H-pvrazolo[3,4-d]pvrimidine
832717-79-0P, 1-(4-Fluoro-6-methoxypyridin-3-v1)-4-[4-(3-isopropyl-
[1,2,4]oxadiazol-5-yl)cyclohexyloxy]-1H-pyrazolo[3,4-d]pyrimidine
832717-80-3P, 4-[4-(3-Isopropyl-[1,2,4]oxadiazol-5-yl)cyclohexyloxy]-1-(6-
methoxy-2-methylpyridin-3-yl)-1H-pyrazolo[3,4-d]pyrimidine
                                                             832717-81-4P.
2,5-Difluoro-4-[4-[4-(3-isopropyl-[1,2,4]oxadiazol-5-
v1)cvclohexvloxvlpvrazolo[3,4-d]pvrimidin-1-v1]benzenesulfonamide
832717-82-5P, 4-[[1-(2-Fluoro-4-methoxyphenyl)-1H-pyrazolo[3,4-d]pyrimidin-
4-vlloxylpiperidine-1-carboxylic acid isopropyl ester
                                                       832717-83-6P.
4-[[1-(4-Difluoromethoxy-2-fluorophenyl)-1H-pyrazolo[3,4-d]pyrimidin-4-
yl]oxy]piperidine-1-carboxylic acid isopropyl ester
                                                      832717-84-7P,
4-[[1-(2-Fluoro-4-trifluoromethoxyphenyl]-1H-pyrazolo[3,4-d]pyrimidin-4-
                                                     832717-85-8P,
vl]oxv]piperidine-1-carboxvlic acid isopropvl ester
4-[[1-(2,5-Difluoro-4-methoxyphenyl)-1H-pyrazolo[3,4-d]pyrimidin-4-
yl]oxy]piperidine-1-carboxylic acid isopropyl ester
                                                     832717-86-9P.
3-Fluoro-4-[4-[[1-(3-isopropyl-[1,2,4]oxadiazol-5-yl)piperidin-4-
yl]oxy]pyrazolo[3,4-d]pyrimidin-1-yl]phenol
                                             832717-87-0P.
1-(2-Fluoro-4-methoxyphenyl)-4-[[1-(3-isopropyl-[1,2,4]oxadiazol-5-
yl)piperidin-4-yl]oxy]-1H-pyrazolo[3,4-d]pyrimidine 832717-88-1P,
1-(4-Difluoromethoxy-2-fluorophenyl)-4-[[1-(3-isopropyl-[1,2,4]oxadiazol-5-
v1)piperidin-4-y1]oxy]-1H-pyrazolo[3,4-d]pyrimidine 832717-89-2P,
1-(2-Fluoro-4-trifluoromethoxyphenyl)-4-[[1-(3-isopropyl-[1,2,4]oxadiazol-
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5-y1)piperidin-4-y1]oxy]-1H-pyrazolo[3,4-d]pyrimidine 832717-90-5P,
1-(2,5-Difluoro-4-methoxyphenyl)-4-[[1-(3-isopropyl-[1,2,4]oxadiazol-5-
v1)piperidin-4-v1|oxv|-1H-pyrazolo[3,4-d]pyrimidine
                                                    832717-91-6P,
3-Fluoro-4-[4-[4-(3-isopropyl-[1,2,4]oxadiazol-5-
yl)cyclohexyloxy]pyrazolo[3,4-d]pyrimidin-1-yl]phenol
                                                      832717-92-7P.
1-(2-Fluoro-4-methoxyphenyl)-4-[4-(3-isopropyl-[1,2,4]oxadiazol-5-
yl)cyclohexyloxy]-1H-pyrazolo[3,4-d]pyrimidine 832717-93-8P,
1-(4-Difluoromethoxy-2-fluoropheny1)-4-[4-(3-isopropy1-[1,2,4]oxadiazol-5-
v1)cvclohexvloxv[-1H-pvrazolo[3,4-d]pvrimidine
                                               832717-94-9P,
1-(2-Fluoro-4-trifluoromethoxyphenyl)-4-[4-(3-isopropyl-[1,2,4]oxadiazol-5-
v1)cvclohexvloxvl-1H-pvrazolo[3,4-d]pvrimidine 832717-95-0P,
4-[[9-(2-Fluoro-4-propionylsulfamoylphenyl)-9H-purin-6-ylloxylpiperidine-1-
carboxylic acid isopropyl ester 832717-96-1P,
4-[[9-(4-Cyano-2-fluorophenyl)-9H-purin-6-yl]oxy[piperidine-1-carboxylic
acid isopropyl ester 832717-97-2P,
4-[[9-(2-Fluoro-4-sulfamoylphenyl)-9H-purin-6-yl]oxy]piperidine-1-
carboxylic acid isopropyl ester 832717-98-3P,
9-(2-Fluoro-4-methylsulfonylphenyl)-6-[[1-(3-isopropyl-[1,2,4]oxadiazol-5-
yl)piperidin-4-yl]oxy]-9H-purine 832717-99-4P,
3-Fluoro-4-[6-[[1-(3-isopropyl-[1,2,4]oxadiazol-5-yl)piperidin-4-
v1]oxv[purin-9-v1]-N-propionvlbenzenesulfonamide 832718-00-0P,
3-Fluoro-4-[6-[[1-(3-isopropyl-[1,2,4]oxadiazol-5-v1)piperidin-4-
vlloxvlpurin-9-vllbenzonitrile
                               832718-01-1P,
3-Fluoro-4-[6-[[1-(3-isopropyl-[1,2,4]oxadiazol-5-yl)piperidin-4-
yl]oxy]purin-9-yl]benzenesulfonamide
                                     832718-02-2P.
4-[[9-(2,5-Difluoro-4-methylsulfonylphenyl)-9H-purin-6-yl]oxy[piperidine-1-
                                832718-03-3P,
carboxylic acid isopropyl ester
4-[[9-(4-Fluoro-6-methoxypyridin-3-v1)-9H-purin-6-v1]oxy|piperidine-1-
carboxylic acid isopropyl ester
                                 832718-04-4P,
4-[[9-(6-Methoxy-2-methylpyridin-3-yl)-9H-purin-6-yl]oxy|piperidine-1-
carboxylic acid isopropyl ester 832718-05-5P,
4-[[9-(2,5-Difluoro-4-sulfamoylphenyl)-9H-purin-6-yl]oxy]piperidine-1-
carboxylic acid isopropyl ester
                                 832718-06-6P,
9-(2,5-Difluoro-4-methylsulfonylphenyl)-6-[[1-(3-isopropyl-
[1,2,4]oxadiazol-5-yl)piperidin-4-yl]oxy]-9H-purine 832718-07-7P,
9-(4-Fluoro-6-methoxypyridin-3-yl)-6-[[1-(3-isopropyl-[1,2,4]oxadiazol-5-
yl)piperidin-4-yl]oxy]-9H-purine
                                 832718-08-8P,
6-[[1-(3-Isopropyl-[1,2,4]oxadiazol-5-yl)piperidin-4-yl]oxy]-9-(6-methoxy-
2-methylpyridin-3-yl)-9H-purine
                                832718-09-9P,
2,5-Difluoro-4-[6-[[1-(3-isopropyl-[1,2,4]oxadiazol-5-v1)piperidin-4-
yl]oxy]purin-9-yl]benzenesulfonamide
                                     832718-10-2P,
9-(2-Fluoro-4-methylsulfonylphenyl)-6-[4-(3-isopropyl-[1,2,4]oxadiazol-5-
vl)cvclohexvloxvl-9H-purine 832718-11-3P.
3-Fluoro-4-[6-[4-(3-isopropyl-[1,2,4]oxadiazol-5-yl)cyclohexyloxy]purin-9-
vl]-N-propionylbenzenesulfonamide
                                   832718-12-4P,
3-Fluoro-4-[6-[4-(3-isopropyl-[1,2,4]oxadiazol-5-yl)cyclohexyloxy]purin-9-
yl]benzonitrile
                 832718-13-5P, 3-Fluoro-4-[6-[4-(3-isopropyl-
[1,2,4]oxadiazol-5-vl)cvclohexvloxvlpurin-9-vl]benzenesulfonamide
832718-14-6P, 9-(2,5-Difluoro-4-methylsulfonylphenyl)-6-[4-(3-isopropyl-
[1,2,4]oxadiazol-5-yl)cyclohexyloxy]-9H-purine
                                               832718-15-7P.
9-(4-Fluoro-6-methoxypyridin-3-y1)-6-[4-(3-isopropyl-[1,2,4]oxadiazol-5-
vl)cvclohexvloxv]-9H-purine
                             832718-16-8P,
6-[4-(3-Isopropyl-[1,2,4]oxadiazol-5-yl)cyclohexyloxy]-9-(6-methoxy-2-
methylpyridin-3-yl)-9H-purine 832718-17-9P,
2,5-Difluoro-4-[6-[4-(3-isopropyl-[1,2,4]oxadiazol-5-
yl)cyclohexyloxy]purin-9-yl]benzenesulfonamide 832718-18-0P,
3-(2-Fluoro-4-methylsulfonylphenyl)-7-[[1-(3-isopropyl-[1,2,4]oxadiazol-5-
yl)piperidin-4-yl]oxy]-3H-[1,2,3]triazolo[4,5-d]pyrimidine 832718-19-1P,
3-Fluoro-4-[7-[[1-(3-isopropyl-[1,2,4]oxadiazol-5-yl)piperidin-4-yl]oxy]-
[1,2,3]triazolo[4,5-d]pyrimidin-3-yl]-N-propionylbenzenesulfonamide
832718-20-4P, 3-Fluoro-4-[7-[[1-(3-isopropy1-[1,2,4]oxadiazo1-5-
yl)piperidin-4-yl]oxy]-[1,2,3]triazolo[4,5-d]pyrimidin-3-yl]benzonitrile
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832718-21-5P, 3-Fluoro-4-[7-[[1-(3-isopropyl-[1,2,4]oxadiazol-5-
v1)piperidin-4-v1]oxv]-[1,2,3]triazolo[4,5-d]pyrimidin-3-
                       832718-22-6P,
vl|benzenesulfonamide
3-(2-Fluoro-4-methylsulfonylphenyl)-7-[4-(3-isopropyl-[1,2,4]oxadiazol-5-
v1)cvclohexvloxv1-3H-[1,2,3]triazolo[4,5-d]pvrimidine 832718-23-7P,
3-Fluoro-4-[7-[4-(3-isopropyl-[1,2,4]oxadiazol-5-yl)cyclohexyloxy]-
[1,2,3]triazolo[4,5-d]pyrimidin-3-y1]-N-propionylbenzenesulfonamide
832718-24-8P, 3-Fluoro-4-[7-[4-(3-isopropyl-[1,2,4]oxadiazol-5-
v1)cvclohexvloxv[-[1,2,3]triazolo[4,5-d]pvrimidin-3-v1]benzonitrile
832718-25-9P, 3-Fluoro-4-[7-[4-(3-isopropyl-[1,2,4]oxadiazol-5-
yl)cyclohexyloxy]-[1,2,3]triazolo[4,5-d]pyrimidin-3-yl]benzenesulfonamide
832718-26-0P, 3-(2,5-Difluoro-4-methylsulfonylphenyl)-7-[4-(3-isopropyl-
[1,2,4]oxadiazol-5-yl)cyclohexyloxy]-3H-[1,2,3]triazolo[4,5-d]pyrimidine
832718-27-1P, 3-(4-Fluoro-6-methoxypyridin-3-yl)-7-[4-(3-isopropyl-
[1,2,4]oxadiazol-5-yl)cyclohexyloxy]-3H-[1,2,3]triazolo[4,5-d]pyrimidine
832718-28-2P, 7-[4-(3-Isopropyl-[1,2,4]oxadiazol-5-yl)cyclohexyloxy]-3-(6-
methoxy-2-methylpyridin-3-yl)-3H-[1,2,3]triazolo[4,5-d]pyrimidine
832718-29-3P, 2,5-Difluoro-4-[7-[4-(3-isopropyl-[1,2,4]oxadiazol-5-
yl)cyclohexyloxy]-[1,2,3]triazolo[4,5-d]pyrimidin-3-yl]benzenesulfonamide
832718-30-6P, 4-[[3-(2-Fluoro-4-methylsulfonylphenyl)-3H-
[1,2,3]triazolo[4,5-d]pyrimidin-7-yl]oxy|piperidine-1-carboxylic acid
isopropyl ester
                 832718-31-7P, 4-113-(2-Fluoro-4-
propionylsulfamovlphenyl)-3H-[1,2,3]triazolo[4,5-d]pyrimidin-7-
vlloxylpiperidine-1-carboxylic acid isopropyl ester 832718-32-8P.
4-[[3-(4-Cyano-2-fluorophenyl)-3H-[1,2,3]triazolo[4,5-d]pyrimidin-7-
vl]oxy|piperidine-1-carboxylic acid isopropyl ester 832718-33-9P,
4-[[3-(2-Fluoro-4-sulfamoylphenyl)-3H-[1,2,3]triazolo[4,5-d]pyrimidin-7-
vl|oxv|piperidine-1-carboxvlic acid isopropvl ester 832718-34-0P,
4-[[3-(2,5-Difluoro-4-methylsulfonylphenyl)-3H-[1,2,3]triazolo[4,5-
d|pyrimidin-7-vlloxy|piperidine-1-carboxylic acid isopropyl ester
832718-35-1P, 4-[[3-(4-Fluoro-6-methoxypyridin-3-y1)-3H-
[1,2,3]triazolo[4,5-d]pyrimidin-7-yl]oxy]piperidine-1-carboxylic acid
isopropyl ester 832718-36-2P, 4-[[3-(6-Methoxy-2-methylpyridin-3-yl)-3H-
[1,2,3]triazolo[4,5-d]pyrimidin-7-yl]oxy]piperidine-1-carboxylic acid
                 832718-37-3P, 4-[[3-(2,5-Difluoro-4-sulfamoylphenyl)-3H-
isopropyl ester
[1,2,3]triazolo[4,5-d]pyrimidin-7-yl]oxy]piperidine-1-carboxylic acid
isopropyl ester 832718-38-4P, 3-(2,5-Difluoro-4-methylsulfonylphenyl)-7-
[[1-(3-isopropyl-[1,2,4]oxadiazol-5-yl)piperidin-4-yl]oxy]-3H-
[1,2,3]triazolo[4,5-d]pyrimidine
                                 832718-39-5P,
3-(4-Fluoro-6-methoxypyridin-3-yl)-7-[[1-(3-isopropyl-[1,2,4]oxadiazol-5-
vl)piperidin-4-vl]oxv]-3H-[1,2,3]triazolo[4,5-d]pvrimidine
                                                           832718-40-8P,
7-[[1-(3-Isopropyl-[1,2,4]oxadiazol-5-yl]piperidin-4-yl]oxyl-3-(6-methoxy-
2-methylpyridin-3-yl)-3H-[1,2,3]triazolo[4,5-d]pyrimidine
2,5-Difluoro-4-[7-[[1-(3-isopropyl-[1,2,4]oxadiazol-5-yl)piperidin-4-
vl]oxy]-[1,2,3]triazolo[4,5-d]pyrimidin-3-yl]benzenesulfonamide
832718-42-0P, 4-[[8-(2-Fluoro-4-methylsulfonylphenyl)-[1,7]naphthyridin-4-
vl]oxv|piperidine-1-carboxvlic acid isopropvl ester
                                                    832718-43-1P,
4-[[8-(2-Fluoro-4-methylsulfonylphenyl)quinolin-4-yl]oxylpiperidine-1-
carboxylic acid isopropyl ester
                                 832718-44-2P.
4-[[8-(2-Fluoro-4-propionylsulfamoylphenyl)quinolin-4-yl]oxy]piperidine-1-
carboxvlic acid isopropyl ester
                                 832718-45-3P,
4-[8-(4-Cyano-2-fluorophenyl)quinolin-4-yloxy|piperidine-1-carboxylic acid
                  832718-46-4P, 4-[8-(2-Fluoro-4-sulfamovlphenvl)guinolin-
isopropyl ester
4-vloxylpiperidine-1-carboxylic acid isopropyl ester 832718-47-5P.
4-[[8-(2,5-Difluoro-4-methylsulfonylphenyl)quinolin-4-yl]oxy]piperidine-1-
carboxylic acid isopropyl ester
                                 832718-48-6P,
4-[8-(4-Fluoro-6-methoxypyridin-3-y1)guinolin-4-yloxy]piperidine-1-
carboxylic acid isopropyl ester 832718-49-7P,
4-[8-(6-Methoxy-2-methy1pyridin-3-y1)quinolin-4-yloxy]piperidine-1-
carboxylic acid isopropyl ester 832718-50-0P,
4-[8-(2,5-Difluoro-4-sulfamoylphenyl)quinolin-4-yloxy]piperidine-1-
carboxylic acid isopropyl ester 832718-51-1P,
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2,5-Difluoro-4-[4-[[1-(3-isopropyl-[1,2,4]oxadiazol-5-yl)piperidin-4-
    v1]oxy]quinolin-8-v1]benzenesulfonamide 832718-52-2P,
    4-[[1-(3-Isopropy1-[1,2,4]oxadiazo1-5-y1)piperidin-4-y1]oxy]-8-(6-methoxy-
    2-methylpyridin-3-vl)quinoline 832718-53-3P,
    8-(4-Fluoro-6-methoxypyridin-3-v1)-4-[[1-(3-isopropyl-[1,2,4]oxadiazol-5-
    yl)piperidin-4-yl]oxy]quinoline 832718-54-4P,
    8-(2,5-Difluoro-4-methylsulfonylphenyl)-4-[[1-(3-isopropyl-
    [1,2,4]oxadiazol-5-yl)piperidin-4-yl]oxy]quinoline 832718-55-5P,
    3-Fluoro-4-[4-[1-(3-isopropyl-[1,2,4]oxadiazol-5-v1)piperidin-4-
    vlloxylguinolin-8-vllbenzenesulfonamide 832718-56-6P,
    3-Fluoro-4-[4-[[1-(3-isopropyl-[1,2,4]oxadiazol-5-yl)piperidin-4-
    yl]oxy]quinolin-8-yl]benzonitrile 832718-57-7P,
    3-Fluoro-4-[4-[[1-(3-isopropyl-[1,2,4]oxadiazol-5-yl)piperidin-4-
    vl]oxy]quinolin-8-vl]-N-propionylbenzenesulfonamide 832718-58-8P
, 8-(2-Fluoro-4-methylsulfonylphenyl)-4-[[1-(3-isopropyl-[1,2,4]oxadiazol-5-
    yl)piperidin-4-yl]oxy]quinoline 832718-59-9P,
    2,5-Difluoro-4-[4-[4-(3-isopropyl-[1,2,4]oxadiazol-5-
    yl)cyclohexyloxy]quinolin-8-yl]benzenesulfonamide
                                                       832718-60-2P.
    4-[4-(3-Isopropy1-[1,2,4]oxadiazo1-5-yl)cyclohexyloxy]-8-(6-methoxy-2-
    methylpyridin-3-yl)quinoline 832718-61-3P,
    8-(4-Fluoro-6-methoxypyridin-3-v1)-4-[4-(3-isopropyl-[1,2,4]oxadiazol-5-
    vl)cvclohexvloxvlguinoline 832718-62-4P,
    8-(2,5-Difluoro-4-methylsulfonylphenyl)-4-(4-(3-isopropyl-(1,2,4)oxadiazol-
    5-v1)cvclohexvloxvlguinoline 832718-63-5P.
    3-Fluoro-4-[4-[4-(3-isopropyl-[1,2,4]oxadiazol-5-yl)cyclohexyloxy]quinolin-
    8-vllbenzenesulfonamide
                             832718-65-7P.
    3-Fluoro-4-[4-[4-(3-isopropyl-[1,2,4]oxadiazol-5-yl)cyclohexyloxy]quinolin-
    8-yl]benzonitrile 832718-67-9P, 3-Fluoro-4-[4-[4-(3-isopropyl-
    [1,2,4]oxadiazol-5-vl)cvclohexvloxvlguinolin-8-vl]-N-
    propionvlbenzenesulfonamide 832718-68-0P.
    8-(2-Fluoro-4-methylsulfonylphenyl)-4-[4-(3-isopropyl-[1,2,4]oxadiazol-5-
    yl)cyclohexyloxy]quinoline 832718-69-1P,
    4-[[8-(2-Fluoro-4-methylsulfonylphenyl)pyrido[3,4-d]pyrimidin-4-
                                                         832718-70-4P,
    yl]oxy]piperidine-1-carboxylic acid isopropyl ester
    4-[[8-(2-Fluoro-4-propionylsulfamoylphenyl)pyrido[3,4-d]pyrimidin-4-
    yl]oxy]piperidine-1-carboxylic acid isopropyl ester
                                                          832718-72-6P,
    4-[[8-(4-Cyano-2-fluorophenyl)pyrido[3,4-d]pyrimidin-4-yl]oxy]piperidine-1-
    carboxylic acid isopropyl ester
                                     832718-74-8P,
    4-[[8-(2-Fluoro-4-sulfamoylphenyl)pyrido[3,4-d]pyrimidin-4-
    vl]oxv]piperidine-1-carboxvlic acid isopropvl ester
                                                          832718-75-9P,
    4-[[8-(2,5-Difluoro-4-methylsulfonylphenyl)pyrido[3,4-d]pyrimidin-4-
    vlloxylpiperidine-1-carboxylic acid isopropyl ester
                                                          832718-76-0P,
    4-[[8-(4-Fluoro-6-methoxypyridin-3-yl)pyrido[3,4-d]pyrimidin-4-
    yl]oxy]piperidine-1-carboxylic acid isopropyl ester
                                                          832718-77-1P.
    4-[[8-(6-Methoxy-2-methylpyridin-3-yl)pyrido[3,4-d]pyrimidin-4-
    vl]oxy|piperidine-1-carboxylic acid isopropyl ester
                                                         832718-78-2P,
    4-[[8-(2,5-Difluoro-4-sulfamovlphenvl)pvrido[3,4-d]pvrimidin-4-
    vlloxylpiperidine-1-carboxylic acid isopropyl ester
                                                         832718-79-3P,
    8-(2-Fluoro-4-methylsulfonylphenyl)-4-[[1-(3-isopropyl-[1,2,4]oxadiazol-5-
    yl)piperidin-4-yl]oxy]pyrido[3,4-d]pyrimidine
                                                    832718-80-6P.
    3-Fluoro-4-[4-[[1-(3-isopropyl-[1,2,4]oxadiazol-5-yl)piperidin-4-
    vl]oxy]pyrido[3,4-d]pyrimidin-8-yl]-N-propionylbenzenesulfonamide
    832718-81-7P, 3-Fluoro-4-[4-[[1-(3-isopropyl-[1,2,4]oxadiazol-5-
    yl)piperidin-4-yl]oxy]pyrido[3,4-d]pyrimidin-8-yl]benzonitrile
    832718-82-8P, 3-Fluoro-4-[4-[[1-(3-isopropyl-[1,2,4]oxadiazol-5-
    yl)piperidin-4-yl]oxy]pyrido[3,4-d]pyrimidin-8-yl]benzenesulfonamide
    832718-83-9P, 8-(2,5-Difluoro-4-methylsulfonylphenyl)-4-[[1-(3-isopropyl-
    [1,2,4]oxadiazol-5-yl)piperidin-4-yl]oxy]pyrido[3,4-d]pyrimidine
    832718-84-0P, 8-(4-Fluoro-6-methoxypyridin-3-y1)-4-[[1-(3-isopropy1-
    [1,2,4]oxadiazol-5-yl)piperidin-4-yl]oxy]pyrido[3,4-d]pyrimidine
    832718-85-1P, 4-[[1-(3-Isopropyl-[1,2,4]oxadiazol-5-yl)piperidin-4-yl]oxy]-
    8-(6-methoxy-2-methylpyridin-3-yl)pyrido[3,4-d]pyrimidine 832718-86-2P,
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2,5-Difluoro-4-[4-[[1-(3-isopropyl-[1,2,4]oxadiazol-5-yl)piperidin-4-
v1|oxy|pyrido[3,4-d|pyrimidin-8-y1|benzenesulfonamide 832718-87-3P,
8-(2-Fluoro-4-methylsulfonylphenyl)-4-[4-(3-isopropyl-[1,2,4]oxadiazol-5-
yl)cyclohexyloxylpyrido[3,4-d]pyrimidine 832718-88-4P,
3-Fluoro-4-[4-[4-[4-(3-isopropv1-[1,2,4]oxadiazol-5-
v1)cyclohexyloxy]pyrido[3,4-d]pyrimidin-8-y1]-N-
propionylbenzenesulfonamide 832718-89-5P,
3-Fluoro-4-[4-[4-(3-isopropyl-[1,2,4]oxadiazol-5-
v1)cvclohexvloxv|pvrido[3,4-d|pvrimidin-8-v1]benzonitrile 832718-90-8P,
3-Fluoro-4-[4-[4-(3-isopropyl-[1,2,4]oxadiazol-5-
yl)cyclohexyloxy]pyrido[3,4-d]pyrimidin-8-yl]benzenesulfonamide
832718-91-9P, 3-(2,5-Difluoro-4-methylsulfonylphenyl)-4-[4-(3-isopropyl-
[1,2,4]oxadiazol-5-yl)cyclohexyloxy]pyrido[3,4-d]pyrimidine
832718-92-0P, 8-(4-Fluoro-6-methoxypyridin-3-yl)-4-[4-(3-isopropyl-
[1,2,4]oxadiazol-5-yl)cyclohexyloxy]pyrido[3,4-d]pyrimidine
832718-93-1P, 4-[4-(3-Isopropyl-[1,2,4]oxadiazol-5-yl)cyclohexyloxy]-8-(6-
methoxy-2-methylpyridin-3-yl)pyrido[3,4-d]pyrimidine
                                                      832718-94-2P.
2,5-Difluoro-4-[4-[4-(3-isopropyl-[1,2,4]oxadiazol-5-
yl)cyclohexyloxy]pyrido[3,4-d]pyrimidin-8-yl]benzenesulfonamide
832718-95-3P, 3-(2-Fluoro-4-methylsulfonylphenyl)-7-[4-(3-isopropyl-
[1,2,4]oxadiazol-5-v1)cvclohexvloxv[pvrazolo[1,5-a]pvrimidine
832718-96-4P, 3-Fluoro-4-[7-[4-(3-isopropyl-[1,2,4]oxadiazol-5-
vl)cvclohexvloxvlpvrazolo[1,5-a]pvrimidin-3-vl]-N-
propionylbenzenesulfonamide
                            832718-97-5P.
3-Fluoro-4-[7-[4-(3-isopropyl-[1,2,4]oxadiazol-5-
vl)cvclohexyloxy[pyrazolo[1,5-a]pyrimidin-3-vl]benzonitrile
832718-98-6P, 3-Fluoro-4-[7-[4-(3-isopropyl-[1,2,4]oxadiazol-5-
v1)cvclohexvloxv|pvrazolo[1,5-a|pvrimidin-3-v1]benzenesulfonamide
832718-99-7P, 3-(2,5-Difluoro-4-methylsulfonylphenyl)-7-(4-(3-isopropyl-
[1,2,4]oxadiazol-5-yl)cyclohexyloxy]pyrazolo[1,5-a]pyrimidine
832719-00-3P, 3-(4-Fluoro-6-methoxypyridin-3-yl)-7-[4-(3-isopropyl-
[1,2,4]oxadiazol-5-yl)cyclohexyloxy]pyrazolo[1,5-a]pyrimidine
832719-01-4P, 7-[4-(3-Isopropyl-[1,2,4]oxadiazol-5-yl)cyclohexyloxy]-3-(6-
methoxy-2-methylpyridin-3-yl)pyrazolo[1,5-a]pyrimidine
                                                        832719-02-5P,
2,5-Difluoro-4-[7-[4-(3-isopropyl-[1,2,4]oxadiazol-5-
yl)cyclohexyloxy]pyrazolo[1,5-a]pyrimidin-3-yl]benzenesulfonamide
832719-03-6P, 4-[[3-(2-Fluoro-4-methylsulfonylphenyl)pyrazolo[1,5-
a]pyrimidin-7-yl]oxy]piperidine-1-carboxylic acid isopropyl ester
832719-04-7P, 4-[(3-(2-Fluoro-4-propionylsulfamoylphenyl)pyrazolo[1,5-
a]pyrimidin-7-yl|oxy|piperidine-1-carboxylic acid isopropyl ester
832719-05-8P, 4-[[3-(4-Cvano-2-fluorophenvl)pvrazolo[1,5-a]pvrimidin-7-
vlloxylpiperidine-1-carboxylic acid isopropyl ester
                                                      832719-06-9P.
4-[[3-(2-Fluoro-4-sulfamoylphenyl)pyrazolo[1,5-a]pyrimidin-7-
yl]oxy]piperidine-1-carboxylic acid isopropyl ester
                                                     832719-07-0P.
4-[[3-(2,5-Difluoro-4-methylsulfonylphenyl)pyrazolo[1,5-a]pyrimidin-7-
vl]oxv|piperidine-1-carboxvlic acid isopropvl ester
                                                     832719-08-1P,
4-[[3-(4-Fluoro-6-methoxypyridin-3-yl)pyrazolo[1,5-a]pyrimidin-7-
                                                      832719-09-2P.
vlloxylpiperidine-1-carboxylic acid isopropyl ester
4-[[3-(6-Methoxy-2-methylpyridin-3-yl)pyrazolo[1,5-a]pyrimidin-7-
vlloxvlpiperidine-1-carboxylic acid isopropyl ester
                                                      832719-10-5P.
4-[[3-(2,5-Difluoro-4-sulfamoylphenyl)pyrazolo[1,5-a]pyrimidin-7-
vl]oxy|piperidine-1-carboxylic acid isopropyl ester
                                                     832719-11-6P,
3-(2-Fluoro-4-methylsulfonylphenyl)-7-[[1-(3-isopropyl-[1,2,4]oxadiazol-5-
yl)piperidin-4-yl]oxy]pyrazolo[1,5-a]pyrimidine
                                                 832719-12-7P.
3-Fluoro-4-[7-[[1-(3-isopropyl-[1,2,4]oxadiazol-5-yl)piperidin-4-
yl]oxy]pyrazolo[1,5-a]pyrimidin-3-yl]-N-propionylbenzenesulfonamide
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
(Uses)
   (drug candidate; preparation of fused aryl and heteroaryl derivs., in
   particular pyrazolopyrimidines, as modulators of G-coupled protein
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receptor and their use in treatment of diabetes, hyperglycemia and

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related diseases)
832719-13-8P, 3-Fluoro-4-[7-[[1-(3-isopropy1-[1,2,4]oxadiazo1-5-
v1)piperidin-4-v1]oxy|pyrazolo[1,5-a|pyrimidin-3-v1]benzonitrile
832719-14-9P, 3-Fluoro-4-[7-[[1-(3-isopropyl-[1,2,4]oxadiazol-5-
yl)piperidin-4-yl]oxy]pyrazolo[1,5-a]pyrimidin-3-yl]benzenesulfonamide
832719-15-0P, 3-(2,5-Difluoro-4-methylsulfonylphenyl)-7-[[1-(3-isopropyl-
[1,2,4]oxadiazol-5-yl)piperidin-4-yl]oxy]pyrazolo[1,5-a]pyrimidine
832719-16-1P, 3-(4-Fluoro-6-methoxypyridin-3-yl)-7-[[1-(3-isopropyl-
[1,2,4]oxadiazol-5-vl)piperidin-4-vl]oxv]pvrazolo[1,5-a]pvrimidine
832719-17-2P, 7-[[1-(3-Isopropyl-[1,2,4]oxadiazol-5-v1)piperidin-4-v1]oxyl-
3-(6-methoxy-2-methylpyridin-3-yl)pyrazolo[1,5-a]pyrimidine
832719-18-3P, 2,5-Difluoro-4-[7-[[1-(3-isopropyl-[1,2,4]oxadiazol-5-
yl)piperidin-4-yl]oxy]pyrazolo[1,5-a]pyrimidin-3-yl]benzenesulfonamide
832719-19-4P, 4-[[3-(2-Fluoro-4-methylsulfonylphenyl)-2-methylpyrazolo[1,5-
a]pyrimidin-7-yl]oxy]piperidine-1-carboxylic acid isopropyl ester
832719-20-7P, 4-[[3-(2-Fluoro-4-propionylsulfamoylphenyl)-2-
methylpyrazolo[1,5-a]pyrimidin-7-yl]oxy]piperidine-1-carboxylic acid
isopropyl ester 832719-21-8P, 4-[[3-(4-Cyano-2-fluorophenyl)-2-
methylpyrazolo[1,5-a]pyrimidin-7-yl]oxy]piperidine-1-carboxylic acid
isopropyl ester 832719-22-9P, 4-[[3-(2-Fluoro-4-sulfamoylphenyl)-2-
methylpyrazolo[1,5-a]pyrimidin-7-yl]oxy|piperidine-1-carboxylic acid
isopropvl ester 832719-23-0P, 4-[[3-(2.5-Difluoro-4-
methylsulfonylphenyl)-2-methylpyrazolo[1,5-a]pyrimidin-7-ylloxylpiperidine-
1-carboxylic acid isopropyl ester 832719-24-1P.
4-[[3-(4-Fluoro-6-methoxypyridin-3-yl)-2-methylpyrazolo[1,5-a]pyrimidin-7-
vl]oxy]piperidine-1-carboxylic acid isopropyl ester 832719-25-2P,
4-[[3-(6-Methoxy-2-methylpyridin-3-yl)-2-methylpyrazolo[1,5-a]pyrimidin-7-
yl]oxy]piperidine-1-carboxylic acid isopropyl ester 832719-26-3P,
4-[3-(2,5-Difluoro-4-sulfamoylphenyl)-2-methylpyrazolo[1,5-a]pyrimidin-7-
yl]oxy]piperidine-1-carboxylic acid isopropyl ester 832719-27-4P,
2,5-Difluoro-4-[7-[[1-(3-isopropyl-[1,2,4]oxadiazol-5-yl)piperidin-4-
yl]oxy]-2-methylpyrazolo[1,5-a]pyrimidin-3-yl]benzenesulfonamide
832719-28-5P, 7-[[1-(3-Isopropyl-[1,2,4]oxadiazol-5-yl)piperidin-4-yl]oxy]-
3-(6-methoxy-2-methylpyridin-3-y1)-2-methylpyrazolo[1,5-a]pyrimidine
832719-29-6P, 3-(4-Fluoro-6-methoxypyridin-3-y1)-7-[[1-(3-isopropyl-
[1,2,4]oxadiazol-5-yl)piperidin-4-yl]oxy]-2-methylpyrazolo[1,5-
alpyrimidine
             832719-30-9P, 3-(2,5-Difluoro-4-methylsulfonylphenyl)-7-[[1-
(3-isopropyl-[1,2,4]oxadiazol-5-yl)piperidin-4-yl]oxy]-2-
methylpyrazolo[1,5-a]pyrimidine
                                832719-31-0P,
3-Fluoro-4-[7-[[1-(3-isopropy1-[1,2,4]oxadiazol-5-yl)piperidin-4-yl]oxy]-2-
                                                       832719-32-1P,
methylpyrazolo[1,5-a]pyrimidin-3-yl]benzenesulfonamide
3-Fluoro-4-[7-[[1-(3-isopropyl-[1,2,4]oxadiazol-5-yl)piperidin-4-yl]oxy]-2-
methylpyrazolo[1,5-a]pyrimidin-3-yl]benzonitrile
                                                  832719-33-2P.
3-Fluoro-4-[7-[[1-(3-isopropyl-[1,2,4]oxadiazol-5-yl)piperidin-4-yl]oxy]-2-
methylpyrazolo[1,5-a]pyrimidin-3-yl]-N-propionylbenzenesulfonamide
832719-34-3P, 3-(2-Fluoro-4-methylsulfonylphenyl)-7-[[1-(3-isopropyl-
[1,2,4]oxadiazol-5-yl)piperidin-4-yl]oxy]-2-methylpyrazolo[1,5-
             832719-35-4P, 3-(2-Fluoro-4-methylsulfonylphenyl)-7-[4-(3-
a]pyrimidine
isopropyl-[1,2,4]oxadiazol-5-yl)cyclohexyloxyl-2-methylpyrazolo[1,5-
              832719-36-5P, 3-Fluoro-4-[7-[4-(3-isopropyl-
alpyrimidine
[1,2,4]oxadiazol-5-yl)cyclohexyloxy]-2-methylpyrazolo[1,5-a]pyrimidin-3-
v1]-N-propionylbenzenesulfonamide
                                  832719-37-6P,
3-Fluoro-4-[7-[4-(3-isopropyl-[1,2,4]oxadiazol-5-yl)cyclohexyloxy]-2-
methylpyrazolo[1,5-a]pyrimidin-3-yl]benzonitrile
                                                  832719-38-7P.
3-Fluoro-4-[7-[4-(3-isopropyl-[1,2,4]oxadiazol-5-yl)cyclohexyloxy]-2-
methylpyrazolo[1,5-a]pyrimidin-3-y1]benzenesulfonamide
                                                        832719-39-8P.
3-(2,5-Difluoro-4-methylsulfonylphenyl)-7-[4-(3-isopropyl-[1,2,4]oxadiazol-
5-y1)cyclohexyloxy]-2-methylpyrazolo[1,5-a]pyrimidine 832719-40-1P,
3-(4-Fluoro-6-methoxypyridin-3-y1)-7-[4-(3-isopropy1-[1,2,4]oxadiazol-5-
yl)cyclohexyloxy]-2-methylpyrazolo[1,5-a]pyrimidine 832719-41-2P,
7-[4-(3-Isopropy1-[1,2,4]oxadiazol-5-yl)cyclohexyloxy]-3-(6-methoxy-2-
methylpyridin-3-y1)-2-methylpyrazolo[1,5-a]pyrimidine 832719-42-3P,
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2,5-Difluoro-4-[7-[4-(3-isopropyl-[1,2,4]oxadiazol-5-yl)cyclohexyloxy]-2-
methylpyrazolo[1,5-a]pyrimidin-3-v1|benzenesulfonamide
                                                        832719-43-4P,
4-[3-(2-Fluoro-4-methylsulfonylphenyl)-1-methyl-1H-pyrazolo[4,3-
d|pvrimidin-7-vl|oxv|piperidine-1-carboxvlic acid isopropvl ester
832719-44-5P, 4-[13-(2-Fluoro-4-propionylsulfamovlphenyl)-1-methyl-1H-
pyrazolo[4,3-d]pyrimidin-7-yl]oxy]piperidine-1-carboxylic acid isopropyl
       832719-45-6P, 4-[[3-(4-Cyano-2-fluorophenyl)-1-methyl-1H-
pyrazolo[4,3-d]pyrimidin-7-yl]oxy[piperidine-1-carboxylic acid isopropyl
       832719-46-7P, 4-||3-(2-Fluoro-4-sulfamovlphenvl)-1-methyl-1H-
pyrazolo[4,3-d]pyrimidin-7-vl]oxy|piperidine-1-carboxylic acid isopropyl
ester 832719-47-8P, 4-113-(2,5-Difluoro-4-methylsulfonylphenyl)-1-methyl-
1H-pyrazolo[4,3-d]pyrimidin-7-yl]oxy]piperidine-1-carboxylic acid
isopropyl ester
                832719-49-0P, 4-[[3-(4-Fluoro-6-methoxypyridin-3-yl)-1-
methyl-1H-pyrazolo[4,3-d]pyrimidin-7-yl]oxy[piperidine-1-carboxylic acid
isopropyl ester 832719-50-3P, 4-[[3-(6-Methoxy-2-methylpyridin-3-y1)-1-
methyl-1H-pyrazolo[4,3-d]pyrimidin-7-yl]oxy]piperidine-1-carboxylic acid
isopropyl ester 832719-52-5P, 4-[[3-(2,5-Difluoro-4-sulfamoylphenyl)-1-
methyl-1H-pyrazolo[4,3-d]pyrimidin-7-yl]oxy]piperidine-1-carboxylic acid
isopropyl ester 832719-54-7P, 3-(2-Fluoro-4-methylsulfonylphenyl)-7-[[1-
(3-isopropyl-[1,2,4]oxadiazol-5-yl)piperidin-4-yl]oxy]-1-methyl-1H-
pyrazolo[4,3-d]pyrimidine 832719-55-8P,
3-Fluoro-4-[7-[\tilde{1}-(3-isopropyl-[1,2,4]oxadiazol-5-yl)piperidin-4-yl]oxy]-1-
methyl-1H-pyrazolo[4,3-d]pyrimidin-3-yl]-N-propionylbenzenesulfonamide
832719-56-9P, 3-Fluoro-4-[7-[[1-(3-isopropyl-[1,2,4]oxadiazol-5-
yl)piperidin-4-yl]oxy]-1-methyl-1H-pyrazolo[4,3-d]pyrimidin-3-
                832719-57-0P, 3-Fluoro-4-[7-[[1-(3-isopropyl-
vllbenzonitrile
[1,2,4]oxadiazol-5-vl)piperidin-4-vl]oxy|-1-methyl-1H-pyrazolo[4,3-
d|pvrimidin-3-v1|benzenesulfonamide
                                    832719-58-1P,
3-(2,5-Difluoro-4-methylsulfonylphenyl)-7-[[1-(3-isopropyl-
[1,2,4]oxadiazol-5-vl)piperidin-4-vl]oxyl-1-methyl-1H-pyrazolo[4,3-
d]pyrimidine 832719-59-2P, 3-(4-Fluoro-6-methoxypyridin-3-y1)-7-[[1-(3-
isopropyl-[1,2,4]oxadiazol-5-yl)piperidin-4-yl]oxy]-1-methyl-1H-
pyrazolo[4,3-d]pyrimidine
                           832719-60-5P,
7-[[1-(3-Isopropyl-[1,2,4]oxadiazol-5-yl)piperidin-4-yl]oxy]-3-(6-methoxy-
2-methylpyridin-3-yl)-1-methyl-1H-pyrazolo[4,3-d]pyrimidine
832719-61-6P, 2,5-Difluoro-4-[7-[[1-(3-isopropyl-[1,2,4]oxadiazol-5-
yl)piperidin-4-yl]oxy]-1-methyl-1H-pyrazolo[4,3-d]pyrimidin-3-
yl]benzenesulfonamide
                       832719-62-7P,
3-(2-Fluoro-4-methylsulfonylphenyl)-7-[4-(3-isopropyl-[1,2,4]oxadiazol-5-
v1)cvclohexyloxy|-1-methyl-1H-pyrazolo[4,3-d]pyrimidine 832719-63-8P,
3-Fluoro-4-[7-[4-(3-isopropyl-[1,2,4]oxadiazol-5-yl)cyclohexyloxy]-1-
methyl-1H-pyrazolo[4,3-d]pyrimidin-3-yl]-N-propionylbenzenesulfonamide
832719-64-9P, 3-Fluoro-4-[7-[4-(3-isopropyl-[9,2,4]oxadiazol-5-
v1)cvclohexvloxvl-1-methyl-1H-pyrazolo[4,3-d]pyrimidin-3-y1]benzonitrile
832719-65-0P, 3-Fluoro-4-[7-[4-(3-isopropyl-[1,2,4]oxadiazol-5-
yl)cyclohexyloxy]-1-methyl-1H-pyrazolo[4,3-d]pyrimidin-3-
vl]benzenesulfonamide
                       832719-66-1P,
3-(2.5-Difluoro-4-methylsulfonylphenyl)-7-[4-(3-isopropyl-[1.2.4]oxadiazol-
5-v1)cvclohexvloxv1-1-methv1-1H-pvrazolo[4,3-d]pvrimidine
                                                           832719-67-2P.
3-(4-Fluoro-6-methoxypyridin-3-yl)-7-[4-(3-isopropyl-[1,2,4]oxadiazol-5-
yl)cyclohexyloxy]-1-methyl-1H-pyrazolo[4,3-d]pyrimidine 832719-68-3P,
7-[4-(3-Isopropyl-[1,2,4]oxadiazol-5-yl)cyclohexyloxy]-3-(6-methoxy-2-
methylpyridin-3-vl)-1-methyl-1H-pyrazolo[4,3-d]pyrimidine 832719-69-4P,
2,5-Difluoro-4-[7-[4-(3-isopropyl-[1,2,4])xadiazol-5-yl)cyclohexyloxy]-1-
methyl-1H-pyrazolo[4,3-d]pyrimidin-3-yl]benzenesulfonamide
                                                            832719-70-7P.
4-[[3-(2-Fluoro-4-methylsulfonylphenyl)-2-methyl-2H-pyrazolo[4,3-
d]pyrimidin-7-yl]oxy]piperidine-1-carboxylic acid isopropyl ester
832719-71-8P, 4-[[3-(2-Fluoro-4-propionylsulfamoylphenyl)-2-methyl-2H-
pyrazolo[4,3-d]pyrimidin-7-yl]oxy]piperidine-1-carboxylic acid isopropyl
       832719-72-9P, 4-[[3-(4-Cyano-2-fluoropheny1)-2-methy1-2H-
pyrazolo[4,3-d]pyrimidin-7-yl]oxy]piperidine-1-carboxylic acid isopropyl
ester 832719-73-0P, 4-[[3-(2-Fluoro-4-sulfamoylphenyl)-2-methyl-2H-
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pyrazolo[4,3-d]pyrimidin-7-yl]oxy]piperidine-1-carboxylic acid isopropyl
       832719-74-1P, 4-[[3-(2,5-Difluoro-4-methylsulfonylphenyl)-2-methyl-
2H-pyrazolo[4,3-d]pyrimidin-7-yl]oxy[piperidine-1-carboxylic acid
isopropyl ester
                832719-75-2P, 4-[[3-(4-Fluoro-6-methoxypyridin-3-y1)-2-
methyl-2H-pyrazolo[4,3-d]pyrimidin-7-yl]oxy]piperidine-1-carboxylic acid
isopropyl ester 832719-76-3P, 4-[[3-(6-Methoxy-2-methylpyridin-3-yl)-2-
methyl-2H-pyrazolo[4,3-d]pyrimidin-7-yl]oxy]piperidine-1-carboxylic acid
isopropyl ester 832719-77-4P, 4-[[3-(2,5-Diffluoro-4-sulfamoylphenyl)-2-
methyl-2H-pyrazolo[4,3-d]pyrimidin-7-yl[oxy]piperidine-1-carboxylic acid
isopropyl ester 832719-78-5P, 3-(2-Fluoro-4-methylsulfonylphenyl)-7-[[1-
(3-isopropyl-[1,2,4]oxadiazol-5-yl)piperidin-4-yl]oxy]-2-methyl-2H-
pyrazolo[4,3-d]pyrimidine 832719-79-6P,
3-Fluoro-4-[7-[[1-(3-isopropyl-[1,2,4]oxadiazol-5-yl)piperidin-4-yl]oxy]-2-
methyl-2H-pyrazolo[4,3-d]pyrimidin-3-yl]-N-propionylbenzenesulfonamide
832719-80-9P, 3-Fluoro-4-[7-[[1-(3-isopropy1-[1,2,4]oxadiazo1-5-
yl)piperidin-4-yl]oxy]-2-methyl-2H-pyrazolo[4,3-d]pyrimidin-3-
yl]benzonitrile 832719-81-0P, 3-Fluoro-4-[7-[[1-(3-isopropyl-
[1,2,4]oxadiazol-5-yl)piperidin-4-yl]oxy]-2-methyl-2H-pyrazolo[4,3-
d]pyrimidin-3-y1]benzenesulfonamide 832719-82-1P,
3-(2,5-Difluoro-4-methylsulfonylphenyl)-7-[[1-(3-isopropyl-
[1,2,4]oxadiazol-5-yl)piperidin-4-yl]oxy]-2-methyl-2H-pyrazolo[4,3-
d]pyrimidine 832719-83-2P, 3-(4-Fluoro-6-methoxypyridin-3-y1)-7-[[1-(3-
isopropyl-[1,2,4]oxadiazol-5-vl)piperidin-4-vl]oxyl-2-methyl-2H-
pyrazolo[4,3-d]pyrimidine 832719-84-3P,
-[[1-(3-Isopropyl-[1,2,4]oxadiazol-5-yl)piperidin-4-yl]oxy]-3-(6-methoxy-
2-methylpyridin-3-yl)-2-methyl-2H-pyrazolo[4,3-d]pyrimidine
832719-85-4P, 2,5-Difluoro-4-[7-[[1-(3-isopropyl-[1,2,4]oxadiazol-5-
v1)piperidin-4-v1|oxv|-2-methv1-2H-pvrazolo[4,3-d]pvrimidin-3-
vllbenzenesulfonamide
                      832719-86-5P,
3-(2-Fluoro-4-methylsulfonylphenyl)-7-[4-(3-isopropyl-[1,2,4]oxadiazol-5-
yl)cyclohexyloxy]-2-methyl-2H-pyrazolo[4,3-d]pyrimidine 832719-87-6P,
3-Fluoro-4-[7-[[4-(3-isopropyl-[1,2,4]-oxadiazol-5-yl)cyclohexyl]oxy]-2-
methyl-2H-pyrazolo[4,3-d]pyrimidin-3-yl]-N-propionylbenzenesulfonamide
832719-88-7P, 3-Fluoro-4-[7-[4-(3-isopropyl-[1,2,4]oxadiazol-5-
yl)cyclohexyloxyl-2-methyl-2H-pyrazolo[4,3-d]pyrimidin-3-yl]benzonitrile
832719-89-8P, 3-Fluoro-4-[7-[4-(3-isopropyl-[1,2,4]oxadiazol-5-
y1)cyclohexyloxy]-2-methy1-2H-pyrazolo[4,3-d]pyrimidin-3-
yl]benzenesulfonamide
                       832719-90-1P,
3-(2,5-Difluoro-4-methylsulfonylphenyl)-7-[4-(3-isopropyl-[1,2,4]oxadiazol-
5-v1)cvclohexyloxy|-2-methyl-2H-pyrazolo[4,3-d]pyrimidine 832719-91-2P,
3-(4-Fluoro-6-methoxypyridin-3-v1)-7-[4-(3-isopropyl-[1,2,4]oxadiazol-5-
v1)cvclohexvloxvl-2-methvl-2H-pvrazolo[4,3-d]pvrimidine 832719-92-3P,
7-[4-(3-Isopropyl-[1,2,4]oxadiazol-5-yl)cyclohexyloxy]-3-(6-methoxy-2-
methylpyridin-3-y1)-2-methyl-2H-pyrazolo[4,3-d]pyrimidine
                                                          832719-93-4P
832721-29-6P
              832721-30-9P
                             832721-31-0P
                                           832721-32-1P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
(Uses)
   (drug candidate; preparation of fused aryl and heteroaryl derivs., in
  particular pyrazolopyrimidines, as modulators of G-coupled protein
  receptor and their use in treatment of diabetes, hyperglycemia and
  related diseases)
35613-84-4P, N-Hydroxvisobutyramidine
                                      49713-38-4P,
2-[(2-Iodophenylamino)methylene|malonic acid diethyl ester
                                                            49713-55-5P,
4-Chloro-8-iodoguinoline
                          51075-37-7P, 1-Cyano-4-hydroxypiperidine
56029-45-9P, 6-tert-Butylnicotinonitrile
                                          106368-32-5P.
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138022-02-3P, 4-[(Methylamino)methyl]piperidine-1-carboxylic acid tert-butyl ester 149806-52-0P, 5'-Bromo-3,4,5,6-tetrahydro-2H-[1,2']bipyridinyl-4-ol 155456-32-9P, 4-[(Acetylamino)methyl]piperidine-1-carboxylic acid tert-butyl ester 205597-70-2P, 8-Iodo-4-oxo-1,4-dihydroquinoline-3-carboxylic acid ethyl

5-Amino-1-(4-methylsulfonylphenyl)-1H-pyrazole-4-carbonitrile

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ester
       329776-71-8P, 4-Methylsulfonylbenzoic acid phenyl ester
606126-17-4P, 3-Fluoro-4-hydrazinobenzenesulfonamide
                                                    614745-80-1P,
4-[(Ethylamino)methyl]piperidine-1-carboxylic acid tert-butyl ester
681508-69-0P, 4-Hydroxy-1-(4-trifluoromethoxyphenyl)piperidine
832714-07-5P, 1-(4-Methylsulfonylphenyl)-1H-pyrazolo[3,4-d]pyrimidin-4-ol
832714-08-6P, 4-Chloro-1-(4-methylsulfonylphenyl)-1H-pyrazolo[3,4-
d]pyrimidine 832714-10-0P, 5-Amino-1-(4-methylsulfonylphenyl)-3-methyl-
1H-pyrazole-4-carbonitrile 832714-11-1P,
1-(4-Methylsulfonylphenyl)-3-methyl-1H-pyrazolo[3,4-d]pyrimidin-4-ol
832714-12-2P, 4-Chloro-1-(4-methylsulfonylphenyl)-3-methyl-1H-pyrazolo[3,4-
d]pyrimidine 832714-14-4P, N-[4-Cyano-2-(4-methylsulfonylphenyl)-5-
methy1-2H-pyrazo1-3-y1]acetamide 832714-15-5P,
1-(4-Methylsulfonylphenyl)-3,6-dimethyl-1,5-dihydropyrazolo[3,4-
d]pyrimidin-4-one 832714-16-6P, 4-Chloro-1-(4-methylsulfonylphenyl)-3,6-
dimethyl-1H-pyrazolo[3,4-d]pyrimidine 832714-37-1P,
1-(3-Isopropyl-[1,2,4]oxadiazol-5-yl)piperidin-4-ol
4-Chloro-1-(2-fluoro-4-methylsulfonylphenyl)-1H-pyrazolo[3,4-d]pyrimidine
832714-47-3P, 5-Amino-1-(2-fluoro-4-methylsulfonylphenyl)-1H-pyrazole-4-
carbonitrile 832714-49-5P, 1-(2-Fluoro-4-methylsulfonylphenyl)-1H-
pyrazolo[3, 4-d]pyrimidin-4-ol 832714-56-4P,
                                          832714-58-6P,
5-Isopropoxymethylpyridine-2-carbonitrile
5-Isopropoxymethylpyridine-2-carboxylic acid 832714-60-0P.
5-Isopropoxypyridine-2-carboxylic acid 832715-03-4P.
5'-Trifluoromethyl-3,4,5,6-tetrahydro-2H-[1,2']bipyridinyl-4-ol
832715-05-6P, 3-Hydroxy-1-[(3-isopropyl-1,2,4-oxadiazol-5-
vl)methyl]pyrrolidine 832715-89-6P,
[1-(4-Methylsulfonylphenyl)-1H-pyrazolo[3,4-d]pyrimidin-4-yl](piperidin-4-
         832715-92-1P, [1-(4-Methylsulfonylphenyl)-1H-pyrazolo[3,4-
vl)amine
dlpvrimidin-4-vll(piperidin-3-vl)amine 832715-99-8P.
6-tert-Butylnicotinic acid 832716-06-0P.
1-[2-(2-Dimethylaminoethoxy)-4-methylsulfonylphenyl]-1H-pyrazolo[3,4-
d]pyrimidin-4-ol 832716-07-1P, [2-[2-(4-Chloropyrazolo[3,4-d]pyrimidin-1-
v1)-5-methylsulfonylphenoxy|ethyl|dimethylamine
                                                 832716-09-3P,
4-(2-Dimethylaminoethylcarbamovl)piperidine-1-carboxylic acid tert-butyl
       832716-10-6P, 4-[(2-Dimethylaminoethylamino)methyl]piperidine-1-
carboxylic acid tert-butyl ester 832716-55-9P
                                                832716-56-0P.
[4-Chloro-1-(4-methylsulfonylphenyl)-1H-pyrazolo[3,4-d]pyrimidin-6-
yl]dimethylamine 832716-59-3P, 1-(2-Dimethylamino-4-
methylsulfonylphenyl)-1H-pyrazolo[3,4-d]pyrimidin-4-ol
4-(Azetidin-3-yloxy)-1-(4-methylsulfonylphenyl)-1H-pyrazolo[3,4-
dlpvrimidine
             832716-91-3P, 1-(2-Fluoro-4-methylsulfonylphenyl)-4-
[(piperidin-4-yl)sulfanyl]-1H-pyrazolo[3,4-d]pyrimidine
                                                        832717-15-4P.
4-[[5-Amino-6-[(4-methylsulfonylphenyl)amino]pyrimidin-4-ylloxylpiperidine-
1-carboxylic acid tert-butyl ester
                                   832717-21-2P,
7-Chloro-3-(4-methylsulfonylphenyl)-3H-[1,2,3]triazolo[4,5-d]pyrimidine
832717-23-4P, 1-(4-Methylsulfonylphenyl)-2-nitroethanone 832717-24-5P,
1-(4-Methylsulfonylphenyl)-2-nitroethanone oxime 832717-25-6P,
3-(4-Methylsulfonylphenyl)-4-nitroisoxazole-5-carboxylic acid ethyl ester
832717-26-7P, 4-Amino-3-(4-methylsulfonylphenyl)isoxazole-5-carboxylic
acid ethyl ester 832717-27-8P, 4-Amino-3-(4-
methylsulfonylphenyl)isoxazole-5-carboxamide
                                             832717-28-9P,
3-(4-Methylsulfonylphenyl)isoxazolo[4,5-d]pyrimidin-7-o1 832717-29-0P,
7-Chloro-3-(4-methylsulfonylphenyl)isoxazolo[4,5-d]pyrimidine
832717-34-7P, 8-Iodo-4-oxo-1,4-dihydroquinoline-3-carboxylic acid
832717-35-8P, 8-Iodo-1H-quinolin-4-one 832717-36-9P,
8-(4-Bromo-2-fluorophenyl)-4-chloroquinoline
                                             832717-38-1P.
4-(8-Chloroquinolin-4-yloxy)piperidine-1-carboxylic acid isopropyl ester
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
   (intermediate; preparation of fused aryl and heteroaryl derivs., in
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particular pyrazolopyrimidines, as modulators of G-coupled protein receptor and their use in treatment of diabetes, hyperglycemia and

related diseases)

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71-41-0, n-Pentanol, reactions 78-82-0, Isobutyronitrile 87-13-8
96-99-1 97-95-0, 2-Ethylbutan-1-ol 100-54-9, 3-Cyanopyridine
108-00-9, N,N-Dimethyl-1,2-ethylenediamine
                                          108-01-0, 2-(
Dimethylamino)ethanol 108-23-6, Isopropyl
chloroformate 109-04-6, 2-Bromopyridine 121-34-6 123-06-8
                                                                402-66-4
407-14-7, 4-(Trifluoromethoxy) bromobenzene 499-05-8 499-81-0,
3,5-Pyridinedicarboxylic acid 503-74-2 535-89-7,
(2-Chloro-6-methylpyrimidin-4-vl)dimethylamine 536-38-9
                                                         536-69-6,
5-Butvlpyridine-2-carboxylic acid 543-27-1, Isobutvl chloroformate
584-02-1, 3-Pentanol 585-70-6, 5-Bromofuran-2-carboxylic acid
592-34-7, n-Butyl chloroformate 615-43-0, 2-Iodoaniline 642-91-1,
2,1-Benzisoxazole-3-carboxylic acid 816-40-0, Bromomethyl ethyl ketone
1072-84-0, 1H-Imidazole-5-carboxylic acid 1219-33-6 1462-86-8,
3-Aminopicolinic acid 2003-10-3 2516-33-8, Cyclopropylmethanol
2566-44-1, 2-Cyclopropylethanol 2632-10-2 3222-47-7 3222-49-9
3222-56-8 3405-77-4 3637-61-4, Cyclopentylmethanol
                                                       4021-13-0,
4-Ethylpyridine-2-carboxylic acid 4052-30-6, 4-Methylsulfonylbenzoic
acid 4415-82-1, Cyclobutylmethanol 4755-77-5, 1-(Chlorocarbonyl)
formic acid ethyl ester 4795-29-3 4837-20-1,
4-Difluoromethoxybenzoic acid 5326-23-8, 6-Chloronicotinic acid 5382-16-1, 4-Hydroxypiperidine 5417-82-3,
                                5469-26-1
1-Ethoxyethylidenemalononitrile
                                            6221-12-1 6313-54-8
6973-60-0 10531-41-6 16331-46-7, 4-Ethoxybenzovl chloride
17852-67-4, 4-(Methylsulfonyl)phenylhydrazine hydrochloride
20260-53-1, Nicotinoyl chloride hydrochloride 20412-38-8, Neopentyl
chloroformate 20826-04-4 21617-12-9, 4,8-Dichloroquinoline
22620-27-5 26095-36-3, 5-[(Morpholin-4-yl)methyl]furan-2-carboxylic acid
36823-88-8, 4-Trifluoromethoxybenzovl chloride
                                               40499-83-0,
3-Hydroxypyrrolidine 41667-95-2 50488-42-1,
2-Bromo-5-trifluoromethylpyridine 52334-81-3,
5-Trifluoromethyl-2-chloropyridine 53939-30-3, 5-Bromo-2-chloropyridine
54042-97-6, 5-Chloromethyl-3-isopropyl-[1,2,4]oxadiazole 60965-26-6
84358-13-4, 1-tert-Butoxycarbonylisonipecotic acid 98546-51-1,
(4-Methylthiophenyl)boronic acid 103057-44-9,
3-Hydroxypyrrolidine-1-carboxylic acid tert-butyl ester 103962-10-3,
2-Bromo-1-(4-trifluoromethoxyphenyl)ethanone
                                            108966-71-8.
3,4-Difluorobenzenesulfonamide 109384-19-2,
4-Hydroxypiperidine-1-carboxylic acid tert-butyl ester 111196-81-7,
2-Chloro-5-ethylpyrimidine 113100-53-1 134464-79-2,
4-Mercaptopiperidine-1-carboxvlic acid tert-butvl ester
144222-22-0, 4-Aminomethylpiperidine-1-carboxylic acid tert-butyl ester
153624-46-5, 4-Isopropoxyphenylboronic acid 175205-81-9,
2-Bromo-4-trifluoromethylpyridine 177759-44-3 195314-59-1,
(4-Aminocyclohexyl)carbamic acid tert-butyl ester 205178-80-9
207986-25-2 210963-95-4 223382-13-6, 1-Benzylazetidin-3-ol
hydrochloride 231291-22-8 253315-22-9 479065-30-0,
1-(2-Methylsulfonylethyl)piperazine
                                    733751-06-9,
(6-Chloro-5-nitropyrimidin-4-yl) (4-methylsulfonylphenyl) amine
832714-22-4, 1-(4-Methylsulfonylphenyl)-4-[(piperidin-4-yl)oxy]-1H-
pyrazolo[3,4-d]pyrimidine hydrochloride 832714-24-6,
1-(2-Fluoro-4-methylsulfonylphenyl)-4-[(piperidin-4-yl)sulfanyl]-1H-
pyrazolo[3,4-d]pyrimidine hydrochloride 832714-35-9,
1-(2-Fluoro-4-methylsulfonylphenyl)-4-[(piperidin-4-yl)oxy]-1H-
pyrazolo[3,4-d]pyrimidine hydrochloride 832714-48-4,
(2-Fluoro-4-methylsulfonylphenyl)hydrazine 832714-57-5,
2-Chloro-5-(isopropoxymethyl)pyridine 832714-62-2,
5'-Isopropoxy-3,4,5,6-tetrahydro-2H-[1,2']bipyridinyl-4-o1 832714-73-5
832715-51-2, 4-Hydroxypiperidine-1-carboxylic acid isopropyl ester
832715-52-3, 1-(4-Bromophenyl)-4-chloro-1H-pyrazolo[3,4-d]pyrimidine
832715-57-8, 4-[[1-(2-Fluoro-4-iodophenyl)-1H-pyrazolo[3,4-d]pyrimidin-4-
yl]oxy]piperidine-1-carboxylic acid isopropyl ester 832715-60-3,
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4-[[1-(4-Iodo-2-methylphenyl)-1H-pyrazolo[3,4-d]pyrimidin-4-
     vl]oxy|piperidine-1-carboxylic acid isopropyl ester
                                                          832715-86-3.
     (3-Fluorophenyl) (4-hydroxypiperidin-1-yl) methanone
                                                         832716-16-2,
     1-[3,5-Bis(trifluoromethyl)phenyl]-4-chloro-1H-pyrazolo[3,4-d]pyrimidine
     832717-00-7 832717-04-1, [1-[(3-Isopropyl-[1,2,4]oxadiazol-5-
                                     832717-08-5,
     yl)methyl]pyrrolidin-3-yl]amine
     [1-(2-Fluoro-4-methylsulfonylphenyl)-1H-pyrazolo[3,4-d]pyrimidin-4-
     vl](pvrrolidin-3-vl)amine
                               832717-16-5,
     4-[[6-[(4-Methylsulfonylphenyl)amino]-5-nitropyrimidin-4-yl]oxylpiperidine-
     1-carboxvlic acid tert-butvl ester 832717-18-7.
     4-[[5-Amino-6-(6-methylsulfonylpyridin-3-ylamino)pyrimidin-4-
     yl]oxy]piperidine-1-carboxylic acid tert-butyl ester
                                                          839732-19-3
     887579-62-6
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (preparation of fused aryl and heteroaryl derivs., in particular
        pyrazolopyrimidines, as modulators of G-coupled protein receptor and
        their use in treatment of diabetes, hyperglycemia and related diseases)
     9004-10-8, Insulin, biological studies
     RL: BSU (Biological study, unclassified); BIOL (Biological study)
        (resistance; preparation of fused anyl and heteroaryl derivs., in particular
        pyrazolopyrimidines, as modulators of G-coupled protein receptor and
        their use in treatment of diabetes, hyperglycemia and related diseases)
     50-99-7, D-Glucose, biological studies
     RL: BSU (Biological study, unclassified); BIOL (Biological study)
        (tolerance; preparation of fused aryl and heteroaryl derivs., in particular
        pyrazolopyrimidines, as modulators of G-coupled protein receptor and
        their use in treatment of diabetes, hyperglycemia and related diseases)
                 833495-64-0 833495-65-1 833495-66-2 833495-67-3
     833495-62-8
     RL: PRP (Properties)
        (unclaimed nucleotide sequence; preparation of fused aryl and heteroaryl
        derivs., in particular pyrazolo[3,4-d]pyrimidines, as modulators of
        G-coupled protein receptor and their use in the prophylaxis and
        treatment of metabolic disorders)
     833495-63-9
     RL: PRP (Properties)
        (unclaimed protein sequence; preparation of fused aryl and heteroaryl
        derivs., in particular pyrazolo[3,4-d]pyrimidines, as modulators of
        G-coupled protein receptor and their use in the prophylaxis and
        treatment of metabolic disorders)
    754986-47-5
     RL: PRP (Properties)
        (unclaimed sequence; preparation of fused aryl and heteroaryl derivs., in
       particular pyrazolo[3,4-d]pyrimidines, as modulators of G-coupled
       protein receptor and their use in the prophylaxis and treatment of
       metabolic disorders)
RE.CNT 26
             THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD
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(2) Anon: WO 0123387 A2 CAPLUS
(3) Anon: WO 0123388 A2 CAPLUS
(4) Anon; WO 02098878 A1 CAPLUS
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(6) Anon; WO 03032989 A1 CAPLUS
(7) Anon: EP 1040831 A2 CAPLUS
(8) Anon: EP 1097709 A2 CAPLUS
(9) Anon: EP 1475094 A1 CAPLUS
(10) Anon; WO 2004000843 A1 CAPLUS
(11) Anon; US 4139705 A CAPLUS
(12) Anon; US 4189579 A CAPLUS
(13) Anon; US 4343804 A CAPLUS
(14) Anon; US 5952504 A CAPLUS
(15) Anon; US 6060478 A CAPLUS
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(16) Anon; JP 61057587 A CAPLUS
(17) Anon; US 6107301 A CAPLUS
(18) Anon; US 6350750 B1 CAPLUS
(19) Anon; US 6506762 B1 CAPLUS
(20) Anon; US 6552192 B1 CAPLUS
(21) Anon; WO 9413677 A1 CAPLUS
(22) Anon; WO 9729109 A1 CAPLUS
(23) Anon; WO 9808846 A1 CAPLUS
(24) Anon; WO 9808847 A1 CAPLUS
(25) Anon: WO 9847874 A1 CAPLUS
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(26) Anon; WO 9951599 A1 CAPLUS

- L9 ANSWER 19 OF 55 CAPLUS COPYRIGHT 2009 ACS on STN
- AN 2004:467862 CAPLUS DN
- 141:38441
- ED Entered STN: 10 Jun 2004
- TI Preparation of N-(carbamimidoylbenzyl)benzeneacetamides and pyridineacetamides as inhibitors of the formation of coagulation factors Xa, IXa, and thrombin induced by factor VIIa and tissue factor
- IN Banner, David William; Gobbi, Luca Claudio; Groebke, Zbinden Katrin; Obst, Ulrike; Stahl, Christoph Martin
- F. Hoffmann-La Roche A.-G., Switz.
- SO PCT Int. Appl., 183 pp. CODEN: PIXXD2
- DT Patent
- LA English
- ΙC ICM C07D213-00 CC
 - 25-19 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds) Section cross-reference(s): 1, 63

FAN.	PA:										APPLICATION NO.									
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	,,,	W:	AE, CO, GH, LR, OM, TN, BW,	AG, CR, GM, LS, PG, TR, GH, KG,	AL, CU, HR, LT, PH, TT, GM, KZ,	AM, CZ, HU, LU, PL, TZ, KE, MD,	AT, DE, ID, LV, PT, UA, LS,	AU, DK, IL, MA, RO, UG, MW, TJ,	AZ, DM, IN, MD, RU, UZ, MZ, TM,	BA, DZ, IS, MG, SC, VC, SD, AT,	EC, JP, MK, SD, VN, SL, BE,	BG, EE, KE, MN, SE, YU, SZ, BG, MC,	EG, KG, MW, SG, ZA, TZ, CH,	ES, KP, MX, SK, ZM, UG, CY,	FI, KR, MZ, SL, ZW, ZM, CZ,	GB, KZ, NI, SY, ZW, DE,	GD, LC, NO, TJ, AM, DK,	GE, LK, NZ, TM, AZ, EE,		
												GQ,								
	CA	2505542				A1	A1 20040610			CA 2003-2505542					20031121					
	AU	2003292072				A1 20040618					AU 2003-292072					20031121				
	AU	2003292072				B2 20061207														
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	EP							EP 2003-767602						20031121						
	EP																			
		R:	AT,	BE,	CH,	DE,	DK,	ES,	FR,	GB,	GR,	IT,	LI,	LU,	NL,	SE,	MC,	PT,		
			IE,	SI,	LT,	LV,	FI,	RO,	MK,	CY,	AL,	TR,	BG,	CZ,	EE,	HU,	SK			
	BR	2003016508				A		20051004		BR 2003-16508					20031121					
	CN	CN 1714079			A		2005	1228		CN 2	N 2003-80103550				20031121					
	JP	P 2006515284 T 384696 S 2298583 O 2005002311				T	T 20060525 T 20080215			CN 2003-80103550 JP 2004-554412 AT 2003-767602					20031121 20031121					
	AT					T														
	ES					13		20080516			ES 2003-767602					20031121				
	NO					A	20050616			ES 2003-767602 NO 2005-2311					20050511					
	MX	2005	0054	46		A		20050826			MX 2005-5446					20050520				
		N 2005CN01009								IN 2005-CN1009					20050524					
PRAI	EP	2002	-263	65		A		2002	1125											

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CLASS PATENT NO.		PATENT FAMILY CLASSIFICATION CODES
WO 2004048335	ICM IPCI IPCR	COTD213-00 COTD213-00 [ICM,7] COTD213-00 [ICM,7] COTD211-00 [I,C,7]; COTD0211-46 [I,A]; COTD0213-00 [I,C,7]; COTD0213-30 [I,A]; COTD0213-38 [I,A]; COTD0213-56 [I,A]; COTD0213-65 [I,A]; COTD0213-73 [I,A]; COTD0239-00 [I,C,7]; COTD0239-42 [I,A]; COTD0265-00 [I,C,7]; COTD0265-36 [I,A]; COTD0271-00 [I,C,7]; COTD0271-06 [I,A]; COTD0295-00 [I,C,7]; COTD0295-15 [I,A]; COTD0310-04 [I,C,7]; COTD02070-01 [I,C,7]; COTD0310-04 [I,A]; COTD02070-01 [I,C,7]; COTD02071-00 [I,C,7]; COTD0310-04 [I,A];
	ECLA	C07D211/46; C07D213/30C; C07D213/38; C07D213/56; C07D213/65; C07D213/65; C07D213/73D; C07D239/42B3; C07D265/36; C07D271/06B; C07D295/14B1F2; C07D309/12; C07D311/04; C07D521/00B2E; M07D;
CA 2505542	IPCI	COTDO213-56 [CDM,7]; COTDO521-00 [ICS,7]; COTDO311-04 [ICS,7]; COTDO311-04 [ICS,7]; COTDO311-06 [ICS,7,C+]; COTDO271-06 [ICS,7]; COTDO271-06 [ICS,7]; COTDO309-12 [ICS,7]; COTDO309-00 [ICS,7,C+]; COTDO309-12 [ICS,7]; COTDO295-00 [ICS,7]; COTDO213-30 [ICS,7]; COTDO213-36 [ICS,7]; COTDO213-30 [ICS,7]; COTDO213-38 [ICS,7]; COTDO213-30 [ICS,7]; COTDO213-36 [ICS,7]; COTDO213-37 [ICS,7]; COTDO213-38 [ICS,7]; COTDO213-38 [ICS,7]; COTDO213-38 [ICS,7]; COTDO213-38 [ICS,7]; COTDO213-39 [ICS,7]; COT
	IPCR ECLA	COTDO211-00 I,c* ; COTDO211-46 I,A ; COTDO213-00 I,C* ; COTDO213-30 I,A ; COTDO213-30 I,A ; COTDO213-36 I,A ; COTDO213-36 I,A ; COTDO213-73 I,A ; COTDO213-56 I,A ; COTDO213-73 I,A ; COTDO253-00 I,C* ; COTDO239-42 I,A ; COTDO251-00 I,C* ; COTDO255-36 I,A ; COTDO271-00 I,C* ; COTDO255-36 I,A ; COTDO271-00 I,C* ; COTDO255-10 I,C* ; COTDO255-10 I,C* ; COTDO255-10 I,C* ; COTDO255-10 I,C* ; COTDO310-00 I,C* ; COTDO310-10 I,C* ;
AU 2003292072	IPCI	COTD521-00B2E COTD521-00 [I.C]; COTD0213-00 [I.A]; COTD0211-00 [I.C*]; COTD0211-46 [I.A]; COTD0213-30 [I.A]; COTD0213-38 [I.A]; COTD0213-65 [I.A]; COTD0213-65 [I.A]; COTD0213-73 [I.A]; COTD0239-00 [I.C*]; COTD0239-42 [I.A]; COTD0265-00 [I.C*]; COTD0265-36 [I.A]; COTD0271-00 [I.C*]; COTD0271-06 [I.A]; COTD0295-00 [I.C*]; COTD0295-15 [I.A]; COTD0399-00 [I.C*]; COTD0309-12 [I.A]; COTD0311-00 [I.C*]; COTD0311-04 [I.A]; COTD0521-00 [I.C*]; COTD0521-00 [I.A]
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C07D0309-00 [ICS, 7,C*1; C07D0311-04 [ICS,7]; C07D0319-00 [ICS,7,C*1; C07D0512-00 [ICS,7]; C07D0512-00 [ICS,7]; C07D0313/30; C07D213/38; C07D213/56; C07D213/30; C07D239/4283; C07D253/65; C07D213/65; C07D213/73D; C07D239/4283; C07D2565/36; C07D211/06B; C07D259/44B1E2; C07D3309/12; C07D311/04; C07D5011-04 [ICM,7]; C07D0211-00 [ICM,7,C*4]

IN 2005CN01009 IPCI OS MARPAT 141:38441

AB Title compds. I [wherein X = O, S, NR12, SO2; Y = N, CR11; R1 = H, OH, NH2, or (un)substituted (arvl)alkoxycarbonyl, arvloxycarbamoyl, alkanoyl, arvlcarbonv1; R2-R4 = independently H, halo, OH, carboxvalkylamino, carbamoylalkylamino, hydroxycycloalkyloxy, (hetero)aryl(oxy), (hetero)aryl(alkyl)amino, etc.; R5 = (cyclo)alkyl; or if X = 0 or NR12, R5 may be H; R6 = H, (fluoro)alkyl; R7-R11 = independently H, OH, halo, NO2, CHO, or (un)substituted amino, fluoroalkyl, alkoxy, (hetero)aryl(oxy), heterocyclylalkyl, carbamoyl, cycloalkyl(alkoxy), etc.; or R8 and R9 or R8 and R7 are bound to each other to form a ring together with the C's to which they are attached; R12 = H, alkyl(carbonyl); and pharmaceutically acceptable salts thereof] were prepared as inhibitors of the formation of coagulation factors Xa, IXa, and thrombin induced by factor VIIa and tissue factor. For example, 6-fluoroveratraldehyde was converted to (2-fluoro-4,5-dimethoxyphenyl)methoxyacetic acid, which was coupled with 4-aminomethylbenzonitrile to give N-(4-cvanobenzyl)-2-(2-fluoro-4,5dimethoxyphenyl)-2-methoxyacetamide. Reaction of the nitrile with dry HCl gas in CHCl3/EtOH afforded the amidine II.HCl. The latter suppressed the amidolytic activity of the factor VIIa/tissue factor complex with Ki of 2.21 μM . Thus, I and their pharmaceutical compns. are useful for the treatment and/or prophylaxis of arterial and venous thrombosis, deep vein thrombosis, pulmonary embolism, unstable angina pectoris, cardiac infarction, stroke due to atrial fibrillation, inflammation, arteriosclerosis, and/or tumors (no data).

II

ST carbamimidoylbenzyl benzeneacetamide pyridineacetamide prepn anticoagulant

thrombolytic antianginal; benzeneacetamide pyridineacetamide carbamimidovlbenzyl prepn coaqulation factor inhibitor Heart, disease (angina pectoris, unstable; preparation of N-(carbamimidovlbenzvl)benzeneacetamides and pyridineacetamides as coagulation factor inhibitors) Thrombosis (arterial; preparation of N-(carbamimidoylbenzyl)benzeneacetamides and pyridineacetamides as coagulation factor inhibitors) Heart, disease (atrial fibrillation, stroke from; preparation of N-(carbamimidovlbenzyl)benzeneacetamides and pyridineacetamides as coagulation factor inhibitors) ΤТ Drug delivery systems (capsules, soft; preparation of N-(carbamimidoylbenzyl)benzeneacetamides and pyridineacetamides as coagulation factor inhibitors) Drug delivery systems (capsules; preparation of N-(carbamimidoylbenzyl)benzeneacetamides and pyridineacetamides as coagulation factor inhibitors) Lung, disease (embolism; preparation of N-(carbamimidovlbenzyl)benzeneacetamides and pyridineacetamides as coagulation factor inhibitors) Anti-inflammatory agents Antianginal agents Antiarteriosclerotics Anticoagulants Antitumor agents Arteriosclerosis Human Inflammation Neoplasm Thrombolytics (preparation of N-(carbamimidovlbenzvl)benzeneacetamides and pyridineacetamides as coagulation factor inhibitors) Blood-coagulation factors RL: BSU (Biological study, unclassified); BIOL (Biological study) (preparation of N-(carbamimidoylbenzyl)benzeneacetamides and pyridineacetamides as coagulation factor inhibitors) Embolism (pulmonary; preparation of N-(carbamimidoylbenzyl)benzeneacetamides and pyridineacetamides as coagulation factor inhibitors) Drug delivery systems

(sachets; preparation of N-(carbamimidoylbenzyl)benzeneacetamides and pyridineacetamides as coagulation factor inhibitors)

Drug delivery systems

(solns., injection; preparation of N-(carbamimidoylbenzyl)benzeneacetamides and pyridineacetamides as coagulation factor inhibitors)

Brain, disease

(stroke, due to atrial fibrillation; preparation of

N-(carbamimidoylbenzyl)benzeneacetamides and pyridineacetamides as

coagulation factor inhibitors)

Drug delivery systems

(tablets, coated; preparation of N-(carbamimidovlbenzvl)benzeneacetamides and pyridineacetamides as coagulation factor inhibitors)

Thrombosis

(venous; preparation of N-(carbamimidoylbenzyl)benzeneacetamides and

pyridineacetamides as coagulation factor inhibitors) 33224-99-6 412271-20-6 793667-52-4 946699-76-9 1055904-44-3 $1055904 - 47 - 6 \qquad 1055904 - 50 - 1 \qquad 1055904 - 51 - 2 \qquad 1055904 - 52 - 3 \qquad 1055904 - 53 - 4 \qquad 1055904 - 53 - 4 \qquad 1055904 - 50 - 2 \qquad 1055904 - 2 \sim 105$ 1055904-58-9 1055904-59-0 1055904-61-4 1055904-64-7 1055904-66-9 $1055904-67-0 \qquad 1055904-69-2 \qquad 1055904-73-8 \qquad 1055904-74-9 \qquad 1055904-76-1$ 1055904-78-3 1055904-80-7 1055904-81-8 1055904-83-0 1055904-85-2

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1055904 - 87 - 4 \qquad 1055904 - 88 - 5 \qquad 1055904 - 91 - 0 \qquad 1055904 - 99 - 8 \qquad 1055905 - 01 - 5
1055905-02-6 1055905-04-8 1055905-06-0 1055905-07-1 1055905-10-6
1055905-11-7
              1055905-12-8 1055905-14-0 1055905-17-3 1055905-18-4
1070987-35-7
RL: PRPH (Prophetic)
   (Preparation of N-(carbamimidoylbenzyl)benzeneacetamides and
   pyridineacetamides as inhibitors of the formation of coaqulation
   factors Xa, IXa, and thrombin induced by factor VIIa and tissue factor)
701263-66-3P, [5-[(4-Carbamimidovlbenzvlcarbamovl)(ethoxy)methvl]-2-
methoxyphenoxylacetic acid ethyl ester hydrochloride
                                                     701263-86-7P,
[4-[(4-Carbamimidovlbenzylcarbamovl) (methoxy)methyllphenoxylacetic acid
methyl ester hydrochloride 701264-67-7P.
N-(4-Carbamimidoylbenzyl)-2-(2,6-difluoro-4-methoxyphenyl)-2-
methoxyacetamide hydrochloride 701265-76-1P,
N-[4-Carbamimidoy1-2-(5-nitropyridin-2-yloxy)benzy1]-2-ethoxy-2-(2-fluoro-
4-methoxyphenyl)acetamide hydrochloride 701265-82-9P,
[5-Carbamimidoy1-2-[[[2-ethoxy-2-(2-fluoro-4-
methoxyphenyl)acetyl]amino]methyl]phenoxy]acetic acid ethyl ester
hydrochloride 701268-14-6P, [[4'-[(4-
Carbamimidoylbenzylcarbamoyl) (ethoxy)methyl]-3',5'-difluorobiphenyl-2-
yl]oxy]acetic acid ethyl ester hydrochloride 701268-43-1P,
4'-[(4-Carbamimidovlbenzylcarbamovl)(ethoxy)methyl]-3',5'-difluorobiphenyl-
3-carboxvlic acid methyl ester hydrochloride 701268-44-2P.
2-[4-(6-Aminopyridin-3-v1)-2.6-difluorophenv1]-N-(4-carbamimidovlbenzv1)-2-
ethoxyacetamide hydrochloride 701268-75-9P.
N-(4-Carbamimidoylbenzyl)-2-(2-ethynyl-6-fluorophenyl)-2-methoxyacetamide
hydrochloride 701268-78-2P, N-(4-Carbamimidoylbenzyl)-2-[2-fluoro-6-(3-
hydroxyprop-1-vnv1)phenv11-2-methoxyacetamide hydrochloride
701269-76-3P, [[5-Carbamimidoyl-2-[[[2-ethoxy-2-(2-fluoro-4-
methoxyphenyl)acetyl]amino]methyl]phenyl]amino]acetic acid ethyl ester
hydrochloride
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic
preparation); THU (Therapeutic use); BIOL (Biological study); PREP
(Preparation); RACT (Reactant or reagent); USES (Uses)
   (anticoagulant; preparation of N-(carbamimidoylbenzyl)benzeneacetamides and
   pyridineacetamides as coagulation factor inhibitors)
701263-28-7P 701263-30-1P 701263-34-5P,
2-(4-Benzyloxyphenyl)-N-(4-carbamimidoylbenzyl)-2-methoxyacetamide
hydrochloride
               701263-37-8P, N-(4-Carbamimidoylbenzyl)-2-methoxy-2-(4-
phenoxyphenyl)acetamide hydrochloride 701263-39-0P,
N-(4-Carbamimidovlbenzvl)-2-methoxy-2-(3-phenoxyphenyl)acetamide
hydrochloride
                701263-41-4P 701263-43-6P,
N-(4-Carbamimidovlbenzvl)-2-(2-fluorophenvl)-2-methoxyacetamide
hydrochloride
               701263-44-7P, 2-(3-Benzyloxyphenyl)-N-(4-
carbamimidoylbenzyl)-2-methoxyacetamide hydrochloride
N-(4-Carbamimidov1benzv1)-2-(3-hydroxyphenv1)-2-methoxyacetamide
                701263-46-9P, N-(4-Carbamimidovlbenzvl)-2-methoxy-2-(3-
hydrochloride
nitrophenyl)acetamide hydrochloride
                                     701263-47-0P.
2-(Biphenyl-4-yl)-N-(4-carbamimidoylbenzyl)-2-methoxyacetamide
                701263-48-1P, 2-(Benzodioxol-5-yl)-N-(4-
hydrochloride
carbamimidoylbenzyl)-2-methoxyacetamide hydrochloride
                                                      701263-49-2P,
2-(Benzodioxol-5-yl)-N-(4-carbamimidoylbenzyl)-2-ethoxyacetamide
                701263-53-8P, N-(4-Carbamimidovlbenzvl)-2-[5-ethoxv-2-
hvdrochloride
fluoro-3-[(1-methylpiperidin-4-yl)oxy]phenyl]-2-methoxyacetamide
hydrochloride 701263-59-4P, 2-(2-Fluoro-4-methoxyphenyl)-N-[4-(N-
aminocarbamimidoyl)benzyl]-2-methoxyacetamide 701263-62-9P,
[5-[(4-Carbamimidoylbenzylcarbamoyl)(methoxy)methyl]-2-
methoxyphenoxy]acetic acid methyl ester hydrochloride
                                                       701263-63-0P.
N-(4-Carbamimidoy1benzy1)-2-[3-(carbamoy1methoxy)-4-methoxypheny1]-2-
methoxyacetamide hydrochloride 701263-67-4P,
N-(4-Carbamimidoy1benzy1)-2-[3-(carbamoy1methoxy)-4-methoxypheny1]-2-
ethoxyacetamide hydrochloride 701263-68-5P,
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[5-[(4-Carbamimidoylbenzylcarbamoyl)(ethoxy)methyl]-2-
methoxyphenoxylacetic acid
                           701263-71-0P,
N-(4-Carbamimidovlbenzyl)-2-ethoxy-2-(4-ethoxyphenyl)acetamide
               701263-73-2P, N-(4-Carbamimidovlbenzvl)-2-methoxv-2-[4-[(1-
hvdrochloride
methylpiperidin-4-yl)oxy[phenyl]acetamide hydrochloride 701263-74-3P,
N-(4-Carbamimidoylbenzyl)-3,3,3-trifluoro-2-methoxy-2-phenylpropionamide
               701263-77-6P, N-(4-Carbamimidoylbenzyl)-2-(2-fluoro-4,5-
hydrochloride
dimethoxyphenyl)-2-methoxyacetamide hydrochloride
                                                  701263-80-1P,
N-(4-Carbamimidovlbenzvl)-2-(3-isopropoxyphenvl)-2-methoxyacetamide
hydrochloride 701263-81-2P, N-(4-Carbamimidovlbenzvl)-2-[4-
(cyclopentyloxy)phenyl1-2-methoxyacetamide hydrochloride 701263-84-5P.
N-(4-Carbamimidoylbenzyl)-2-(4-isopropoxyphenyl)-2-methoxyacetamide
hydrochloride
              701263-87-8P, [4-[(4-
Carbamimidoylbenzylcarbamoyl) (methoxy)methyl|phenoxy|acetic acid
701263-89-0P, N-(4-Carbamimidoylbenzyl)-2-methoxy-2-[3-[(tetrahydropyran-4-
yl)oxy]phenyl]acetamide hydrochloride
                                       701263-92-5P,
N-(4-Carbamimidoylbenzyl)-2-(3,5-diethoxy-2-fluorophenyl)-2-
methoxyacetamide hydrochloride 701263-95-8P,
N-(4-Carbamimidoylbenzyl)-2-[5-ethoxy-2-fluoro-4-(2-hydroxyethoxy)phenyl]-
2-methoxyacetamide hydrochloride 701263-99-2P,
N-(4-Carbamimidovlbenzvl)-2-(3,4-diethoxy-2-fluorophenvl)-2-
methoxyacetamide hydrochloride 701264-02-0P,
N-(4-Carbamimidoy1-2-fluorobenzy1)-2-(2-fluoro-4-methoxypheny1)-2-
methoxyacetamide hydrochloride 701264-04-2P.
N-(4-Carbamimidoy1-3-fluorobenzy1)-2-(2-fluoro-4-methoxypheny1)-2-
methoxyacetamide hydrochloride 701264-05-3P,
2-[2,4-Bis(trifluoromethyl)phenyl]-N-(4-carbamimidoylbenzyl)-2-
methoxyacetamide hydrochloride 701264-11-1P,
N-(4-Carbamimidovlbenzvl)-2-(2-hvdroxv-4-methoxyphenvl)-2-methoxyacetamide
        701264-12-2P, N-(4-Carbamimidoylbenzyl)-2-(2-fluoro-5-
methoxyphenyl)-2-methoxyacetamide hydrochloride
                                                701264-13-3P,
N-(4-Carbamimidoylbenzyl)-2-(2,3-difluorophenyl)-2-methoxyacetamide
              701264-14-4P, N-(4-Carbamimidovlbenzvl)-2-(2,6-
hydrochloride
difluorophenvl)-2-methoxvacetamide hydrochloride
                                                  701264-15-5P,
2-(4-Bromo-2-fluorophenyl)-N-(4-carbamimidoylbenzyl)-2-methoxyacetamide
hydrochloride
               701264-17-7P, 2-(4-Bromo-2-fluorophenyl)-N-(4-
carbamimidoylbenzyl)-2-ethoxyacetamide hydrochloride
                                                     701264-19-9P.
2-(4-Bromo-2-fluorophenyl)-N-(4-carbamimidoylbenzyl)-2-propoxyacetamide
               701264-20-2P, N-(4-Carbamimidoylbenzyl)-2-(2-fluoro-4-
trifluoromethylphenyl)-2-methoxyacetamide hydrochloride 701264-22-4P,
N-(4-Carbamimidovlbenzvl)-2-[4-(2-hydroxyethoxy)phenyl]-2-methoxyacetamide
hydrochloride
               701264-24-6P, N-(4-Carbamimidoylbenzyl)-2-(4-
dimethylaminophenyl)-2-methoxyacetamide hydrochloride
N-(4-Carbamimidoylbenzyl)-2-methoxy-2-(3-oxo-3,4-dihydro-2H-
benzo[1,4]oxazin-6-yl)acetamide hydrochloride
                                               701264-27-9P,
N-(4-Carbamimidoylbenzyl)-2-methoxy-2-[4-(pyrrolidin-1-yl)phenyl]acetamide
               701264-29-1P, N-(4-Carbamimidovlbenzvl)-2-(2-chlorophenvl)-
hydrochloride
2-methoxvacetamide hydrochloride
                                  701264-32-6P.
2-(4-Acetylaminophenyl)-N-(4-carbamimidoylbenzyl)-2-methoxyacetamide
               701264-35-9P, N-(4-Carbamimidoylbenzyl)-2-methoxy-2-(4-
hydrochloride
trifluoromethoxyphenyl)acetamide hydrochloride
                                                701264-37-1P,
N-(4-Carbamimidoylbenzyl)-2-[4-(imidazol-1-yl)phenyl]-2-methoxyacetamide
               701264-40-6P, N-(4-Carbamimidovlbenzvl)-2-methoxy-2-(6-
hvdrochloride
methoxynaphthalen-2-vl)acetamide hydrochloride
                                                701264-42-8P.
N-(4-Carbamimidoylbenzyl)-2-methoxy-2-[4-(morpholin-4-yl)phenyl]acetamide
hydrochloride
               701264-43-9P, N-(4-Carbamimidoylbenzyl)-2-methoxy-2-[2-
(morpholin-4-yl)phenyl]acetamide hydrochloride
                                                701264-45-1P.
N-(4-Carbamimidoylbenzyl)-2-[4-(3-dimethylaminopropoxy)phenyl]-2-
methoxyacetamide hydrochloride 701264-48-4P,
N-(4-Carbamimidoylbenzyl)-2-(4'-dimethylamino-3-fluorobiphenyl-4-yl)-2-
methoxyacetamide hydrochloride 701264-49-5P,
N-(4-Carbamimidoylbenzyl)-2-(3-fluoro-4'-methoxybiphenyl-4-yl)-2-
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methoxyacetamide hydrochloride 701264-50-8P,
N-(4-Carbamimidoy1benzy1)-2-(3-fluoro-2'-methoxybipheny1-4-y1)-2-
methoxyacetamide hydrochloride 701264-51-9P,
N-(4-Carbamimidoylbenzyl)-2-(3-fluorobiphenyl-4-yl)-2-methoxyacetamide
              701264-52-0P, N-(4-Carbamimidoylbenzyl)-2-(3-fluoro-3'-
hvdrochloride
methoxybiphenyl-4-yl)-2-methoxyacetamide hydrochloride 701264-55-3P,
N-(4-Carbamimidoylbenzyl)-2-(2,2-dimethylchroman-6-yl)-2-methoxyacetamide
hydrochloride
               701264-59-7P, 2-Ethoxy-2-(2-fluoro-4-methoxyphenyl)-N-[4-
(N-hydroxycarbamimidovl)benzyllacetamide 701264-61-1P,
4-[3-(3-Cyclopentyloxy-4-methoxyphenyl)-3-methoxy-2-
oxopropyllamino|benzamidine hydrochloride 701264-64-4P.
N-(4-Carbamimidoylbenzyl)-2-(2-chloro-4-methoxyphenyl)-2-methoxyacetamide
hydrochloride
               701264-69-9P, N-(4-Carbamimidoylbenzyl)-2-(2-fluoro-4-
methoxyphenyl)-2-propoxyacetamide hydrochloride
                                               701264-71-3P.
N-(4-Carbamimidoylbenzyl)-2-methoxy-2-(naphthalen-1-yl)propionamide
              701264-73-5P, 2-(4-Bromo-2,6-difluorophenyl)-N-(4-
hydrochloride
carbamimidoylbenzyl)-2-methoxyacetamide hydrochloride 701264-78-0P,
N-(4-Carbamimidoylbenzyl)-2-(2-fluoro-4-isopropoxyphenyl)-2-
methoxyacetamide hydrochloride 701264-80-4P,
N-(4-Carbamimidoylbenzyl)-2-(2-fluoro-4-isobutoxyphenyl)-2-
methoxyacetamide hydrochloride 701264-82-6P,
N-(4-Carbamimidovlbenzvl)-2-[2-fluoro-4-[2-(4-fluorophenvl)ethoxy]phenvl]-
2-methoxyacetamide hydrochloride 701264-85-9P,
N-(4-Carbamimidovlbenzyl)-2-[2-fluoro-4-(pyridin-3-yl)phenyl]-2-
methoxyacetamide hydrochloride 701264-87-1P,
N-(4-Carbamimidoylbenzyl)-2-[2-fluoro-4-(pyridin-4-yl)phenyl]-2-
methoxyacetamide hydrochloride 701264-90-6P,
2-(5-Bromo-2-fluorophenvl)-N-(4-carbamimidovlbenzvl)-2-methoxvacetamide
hvdrochloride
              701264-92-8P, N-(4-Carbamimidovlbenzvl)-2-(4-
fluorobiphenv1-3-v1)-2-methoxyacetamide hydrochloride 701264-95-1P.
N-(4-Carbamimidoylbenzyl)-2-(2-fluoro-5-methylphenyl)-2-methoxyacetamide
hydrochloride
               701264-98-4P, N-(4-Carbamimidoylbenzyl)-2-(2-fluoro-5-
trifluoromethylphenyl)-2-methoxyacetamide hydrochloride 701265-01-2P,
N-(4-Carbamimidovlbenzvl)-2-(2-fluoro-6-methoxyphenyl)-2-methoxyacetamide
              701265-09-0P 701265-11-4P
                                             701265-13-6P 701265-15-8P
hvdrochloride
701265-17-0P
              701265-19-2P 701265-23-8P,
N-(4-Carbamimidoy1benzy1)-2-[2-fluoro-4-(2-phenoxyethoxy)pheny1]-2-
methoxyacetamide hydrochloride 701265-25-0P,
N-(4-Carbamimidoylbenzyl)-2-methoxy-2-(pyridin-2-yl)acetamide
               701265-27-2P, N-(4-Carbamimidovlbenzyl)-2-methoxy-2-
hydrochloride
phenylpropionamide hydrochloride 701265-28-3P,
2-(4-Bromo-2,6-difluorophenyl)-N-(4-carbamimidoylbenzyl)-2-ethoxyacetamide
hydrochloride
               701265-30-7P, N-(4-Carbamimidovlbenzyl)-2-[2-fluoro-6-(2-
hydroxyethoxy)phenyl]-2-methoxyacetamide hydrochloride
                                                       701265-32-9P.
N-(4-Carbamimidoylbenzyl)-2-[2-(carbamoylmethoxy)-6-fluorophenyl]-2-
                  701265-36-3P, 2-(Biphenyl-4-yl)-N-(4-
methoxvacetamide
carbamimidovlbenzvl)-2-ethoxypropionamide hydrochloride
                                                        701265-42-1P.
2-[3-[1-(Benzenesulfonvl)piperidin-4-vloxv]-5-ethoxv-2-fluorophenvl]-N-(4-
carbamimidovlbenzvl)-2-methoxyacetamide hydrochloride
                                                      701265-43-2P.
N-(4-Carbamimidoylbenzyl)-2-[5-ethoxy-2-fluoro-3-[[1-
(methanesulfonyl)piperidin-4-yl]oxy]phenyl]-2-methoxyacetamide
hydrochloride
               701265-44-3P, 2-[3-(1-Acetylpiperidin-4-yloxy)-5-ethoxy-2-
fluorophenvl]-N-(4-carbamimidovlbenzvl)-2-methoxyacetamide hydrochloride
701265-45-4P, 2-[3-(1-Benzoylpiperidin-4-yloxy)-5-ethoxy-2-fluorophenyl]-N-
(4-carbamimidoylbenzyl)-2-methoxyacetamide hydrochloride 701265-47-6P,
N-(4-Carbamimidoy1-2-chlorobenzy1)-2-(2-fluoro-4-methoxypheny1)-2-
methoxyacetamide hydrochloride
                                701265-49-8P,
N-(4-Carbamimidov1-2-chlorobenzv1)-2-ethoxy-2-(2-fluoro-4-
methoxyphenyl)acetamide hydrochloride 701265-54-5P,
N-(4-Carbamimidoy1-2-chlorobenzy1)-2-(2,6-difluoro-4-methoxypheny1)-2-
ethoxyacetamide hydrochloride 701265-56-7P,
N-(4-Carbamimidoy1-2-chlorobenzy1)-2-(2,6-difluoro-4-methoxypheny1)-2-
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methoxyacetamide hydrochloride 701265-60-3P,
N-(4-Carbamimidov1-3-chlorobenzv1)-2-ethoxy-2-(2-fluoro-4-
methoxyphenyl)acetamide acetate 701265-61-4P,
2-(4-Bromo-2,6-difluorophenyl)-N-(4-carbamimidoyl-2-methoxybenzyl)-2-
ethoxyacetamide hydrochloride 701265-63-6P.
N-(4-Carbamimidov1-2-methoxybenzy1)-2-ethoxy-2-(2-fluoro-4-
                                       701265-67-0P.
methoxyphenyl)acetamide hydrochloride
N-(4-Carbamimidoy1-2-phenoxybenzy1)-2-ethoxy-2-(2-fluoro-4-
methoxyphenyl)acetamide hydrochloride
                                       701265-68-1P,
N-[4-Carbamimidov1-2-(o-tolvloxy)benzyl]-2-ethoxy-2-(2-fluoro-4-
methoxyphenyl)acetamide hydrochloride 701265-69-2P,
N-[4-Carbamimidoy1-2-(4-fluorophenoxy)benzy1]-2-ethoxy-2-(2-fluoro-4-
methoxyphenyl)acetamide hydrochloride 701265-71-6P 701265-77-2P,
N-[2-(5-Aminopyridin-2-yloxy)-4-carbamimidoylbenzyl]-2-ethoxy-2-(2-fluoro-
4-methoxyphenyl)acetamide hydrochloride
                                        701265-80-7P,
N-(5-Carbamimidoylbiphenyl-2-ylmethyl)-2-ethoxy-2-(2-fluoro-4-
methoxyphenyl)acetamide hydrochloride
                                      701265-83-0P.
N-[4-Carbamimidoy1-2-(carbamoy1methoxy)benzy1]-2-ethoxy-2-(2-fluoro-4-
methoxyphenyl)acetamide hydrochloride
                                      701265-84-1P,
N-(4-Carbamimidoy1-2-isopropoxybenzy1)-2-ethoxy-2-(2-fluoro-4-
methoxyphenyl)acetamide hydrochloride 701265-85-2P,
N-[4-Carbamimidov1-2-(2-hvdroxvethoxv)benzv1]-2-ethoxv-2-(2-fluoro-4-
methoxyphenyl)acetamide hydrochloride 701265-86-3P 701265-87-4P,
[5-Carbamimidov1-2-[[[2-ethoxy-2-(2-fluoro-4-
methoxyphenyl)acetyllaminolmethyllphenoxylacetic acid
                                                      701265-88-5P
701265-89-6P
             701265-90-9P
                            701265-91-0P 701265-94-3P,
N-[4-Carbamimidoy1-2-(carbamoy1methoxy)benzy1]-2-(2-fluoro-4-
methoxyphenyl)-2-methoxyacetamide hydrochloride 701265-96-5P,
N-(4-Carbamimidoy1-2-phenoxybenzy1)-2-(2,6-difluoro-4-methoxypheny1)-2-
ethoxyacetamide hydrochloride 701265-98-7P.
N-(4-Carbamimidoy1-2-methoxybenzy1)-2-(2,6-difluoro-4-methoxybenv1)-2-
ethoxyacetamide hydrochloride 701266-01-5P,
N-[4-Carbamimidoy1-2-(carbamoylmethoxy)benzy1]-2-(2,6-difluoro-4-
methoxyphenyl)-2-ethoxyacetamide hydrochloride 701266-02-6P,
N-[4-Carbamimidoy1-2-(2-fluorobenzyloxy)benzyl]-2-(2,6-difluoro-4-
methoxyphenyl)-2-ethoxyacetamide hydrochloride 701266-03-7P,
N-[4-Carbamimidoyl-2-(5-chloro-2-fluorobenzyloxy)benzyl]-2-(2,6-difluoro-4-
methoxyphenyl)-2-ethoxyacetamide hydrochloride
                                               701266-04-8P,
N-[4-Carbamimidoy1-2-[(2-methoxyethylcarbamoy1)methoxy]benzy1]-2-(2,6-
difluoro-4-methoxyphenyl)-2-ethoxyacetamide hydrochloride 701266-05-9P,
N-[4-Carbamimidov1-2-[[[2-(morpholin-4-v1)ethv1]carbamov1]methoxv]benzv1]-
2-(2,6-difluoro-4-methoxyphenyl)-2-ethoxyacetamide hydrochloride
701266-06-0P, N-[4-Carbamimidov1-2-[(2-
diethylaminoethylcarbamoyl)methoxy]benzyl]-2-(2,6-difluoro-4-
methoxyphenyl)-2-ethoxyacetamide hydrochloride
                                               701266-07-1P,
N-[4-Carbamimidov1-2-[([1,2,4]oxadiazo1-3-v1)methoxy]benzv1]-2-(2,6-
difluoro-4-methoxyphenyl)-2-ethoxyacetamide hydrochloride
                                                           701266-08-2P.
N-(4-Carbamimidov1-2-carbamimidov1methoxybenzy1)-2-(2,6-difluoro-4-
methoxyphenyl)-2-ethoxyacetamide hydrochloride
                                               701266-09-3P.
N-[2-(1H-Benzimidazol-2-ylmethoxy)-4-carbamimidoylbenzyl]-2-(2,6-difluoro-
4-methoxyphenyl)-2-ethoxyacetamide hydrochloride
                                                  701266-11-7P
701266-13-9P
              701266-14-0P, N-[4-Carbamimidoy1-2-
(carbamoylmethoxy)benzyl]-2-(2,6-difluoro-4-methoxyphenyl)-2-
methoxyacetamide hydrochloride
                               701266-17-3P.
N-[4-Carbamimidov1-2-[(methylcarbamov1)methoxylbenzy1]-2-(2.6-difluoro-4-
methoxyphenyl)-2-methoxyacetamide hydrochloride 701266-18-4P,
N-[4-Carbamimidoy1-2-[(isopropylcarbamoy1)methoxy]benzy1]-2-(2,6-difluoro-
4-methoxyphenyl)-2-methoxyacetamide hydrochloride
                                                   701266-19-5P,
N-[4-Carbamimidoy1-2-[(4-fluorophenylcarbamoy1)methoxy]benzy1]-2-(2,6-
difluoro-4-methoxyphenyl)-2-methoxyacetamide hydrochloride 701266-20-8P,
N-[4-Carbamimidoy1-2-(pyridin-2-ylmethoxy)benzy1]-2-(2,6-difluoro-4-
methoxyphenyl)-2-methoxyacetamide hydrochloride
                                                701266-22-0P.
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N-[4-Carbamimidoy1-2-(2,2,2-trifluoroethoxy)benzy1]-2-(2,6-difluoro-4-
methoxyphenyl)-2-methoxyacetamide hydrochloride 701266-23-1P,
N-[4-Carbamimidoy1-2-(pyridin-3-ylmethoxy)benzy1]-2-(2,6-difluoro-4-
methoxyphenyl)-2-methoxyacetamide hydrochloride 701266-24-2P.
N-[4-Carbamimidov1-2-(pyridin-4-vlmethoxy)benzy1]-2-(2.6-difluoro-4-
methoxyphenyl)-2-methoxyacetamide hydrochloride
                                                701266-31-1P.
N-(4-Carbamimidoylbenzyl)-2-(2,6-difluoro-4-hydroxyphenyl)-2-
ethoxyacetamide hydrochloride 701266-33-3P,
N-(4-Carbamimidovlbenzvl)-2-[2,6-difluoro-4-[2-(morpholin-4-
vl)ethoxylphenvl]-2-ethoxyacetamide dihydrochloride
                                                    701266-34-4P.
N-(4-Carbamimidovlbenzyl)-2-(2,6-difluoro-4-phenethyloxyphenyl)-2-
ethoxyacetamide hydrochloride 701266-35-5P,
N-(4-Carbamimidoylbenzyl)-2-[4-(cyclopropylmethoxy)-2,6-difluorophenyl]-2-
ethoxyacetamide hydrochloride 701266-36-6P,
N-(4-Carbamimidoylbenzyl)-2-ethoxy-2-(4-ethoxy-2,6-
difluorophenyl)acetamide hydrochloride 701266-40-2P,
N-(4-Carbamimidoylbenzyl)-2-[2,6-difluoro-4-(4-methoxyphenoxy)phenyl]-2-
                701266-43-5P, N-(4-Carbamimidoylbenzyl)-2-[4-(3,4-
ethoxyacetamide
dimethoxyphenoxy)-2,6-difluorophenyl]-2-ethoxyacetamide hydrochloride
701266-47-9P, N-(4-Carbamimidoylbenzyl)-2-[2,6-difluoro-4-(3-
methoxyphenoxy)phenyl]-2-ethoxyacetamide hydrochloride
                                                       701266-51-5P,
2-[4-(3-Acetylaminophenoxy)-2,6-difluorophenyl]-N-(4-carbamimidoylbenzyl)-
2-ethoxyacetamide hydrochloride
                                701266-54-8P.
N-(4-Carbamimidovlbenzvl)-2-[4-(4-cyanophenoxy)-2,6-difluorophenvl]-2-
ethoxyacetamide hydrochloride 701266-58-2P.
N-(4-Carbamimidoylbenzyl)-2-(2,6-difluoro-4-(3-
trifluoromethoxyphenoxy)phenyl | -2-ethoxyacetamide hydrochloride
701266-65-1P, 4-[(4-Carbamimidovlbenzylcarbamovl)(ethoxy)methyl]-3,5-
difluoro-N-isobutylbenzamide hydrochloride 701266-66-2P.
4-[(4-Carbamimidoylbenzylcarbamoyl)(ethoxy)methyl]-N-ethyl-3,5-
difluorobenzamide hydrochloride
                                 701266-67-3P,
4-[(4-Carbamimidoylbenzylcarbamoyl)(ethoxy)methyl]-3,5-difluoro-N-(2-
methoxyethyl)benzamide hydrochloride
                                     701266-68-4P,
4-[(4-Carbamimidoylbenzylcarbamoyl)(ethoxy)methyl]-N-cyclopentyl-3,5-
difluorobenzamide hydrochloride
                                 701266-69-5P,
4-[(4-Carbamimidoylbenzylcarbamoyl)(ethoxy)methyl]-3,5-difluoro-N-(2,2,2-
trifluoroethyl) benzamide hydrochloride
                                       701266-70-8P,
4-[(4-Carbamimidoylbenzylcarbamoyl)(ethoxy)methyl]-N-cyclopropylmethyl-3,5-
difluorobenzamide hydrochloride
                                 701266-77-5P,
N-(4-Carbamimidovlbenzvl)-2-(2,6-difluoro-3-hydroxyphenvl)-2-
ethoxyacetamide hydrochloride 701266-78-6P,
N-(4-Carbamimidovlbenzvl)-2-ethoxy-2-[3-[2-(2-ethoxyethoxy)ethoxy]-2,6-
difluorophenyllacetamide hydrochloride 701266-79-7P.
N-(4-Carbamimidoylbenzyl)-2-[3-(3-dimethylaminopropoxy)-2,6-
difluorophenyl]-2-ethoxyacetamide dihydrochloride
                                                   701266-80-0P.
N-(4-Carbamimidovlbenzvl)-2-[2,6-difluoro-3-[2-[2-(2-
methoxyethoxy)ethoxylethoxylphenyl]-2-ethoxyacetamide hydrochloride
701266-81-1P, N-(4-Carbamimidovlbenzvl)-2-[2,6-difluoro-3-[3-(pvridin-4-
vl)propoxylphenvl1-2-ethoxyacetamide dihydrochloride
                                                      701266-82-2P.
N-(4-Carbamimidoylbenzyl)-2-[2,6-difluoro-3-[2-(pyrrolidin-1-
yl)ethoxy[phenyl]-2-ethoxyacetamide dihydrochloride
                                                     701266-83-3P,
N-(4-Carbamimidovlbenzvl)-2-[2,6-difluoro-3-(1-
methylcyclopropylmethoxy)phenyl]-2-ethoxyacetamide hydrochloride
701266-84-4P, N-(4-Carbamimidoylbenzyl)-2-[2,6-difluoro-3-[2-(piperidin-1-
yl)ethoxy]phenyl]-2-ethoxyacetamide dihydrochloride
                                                    701266-85-5P
701266-86-6P, N-(4-Carbamimidoylbenzyl)-2-ethoxy-2-[3-(2-ethoxyethoxy)-2,6-
difluorophenyl]acetamide hydrochloride 701266-87-7P,
N-(4-Carbamimidoy1benzy1)-2-[2,6-dif1uoro-3-(2-methoxyethoxy)pheny1]-2-
ethoxyacetamide hydrochloride 701266-88-8P,
N-(4-Carbamimidoy1benzy1)-2-[3-(3-dimethylamino-2,2-dimethylpropoxy)-2,6-
difluorophenyl]-2-ethoxyacetamide dihydrochloride 701266-89-9P,
N-(4-Carbamimidoylbenzyl)-2-[2,6-difluoro-3-[2-(thiophen-2-
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yl)ethoxy[phenyl]-2-ethoxyacetamide hydrochloride 701266-90-2P
    701266-91-3P, N-(4-Carbamimidoylbenzyl)-2-(2,6-difluoro-3-isobutoxyphenyl)-
                                      701266-92-4P
    2-ethoxyacetamide hydrochloride
                                                     701266-93-5P,
    N-(4-Carbamimidovlbenzyl)-2-[3-(2-cyclopropylethoxy)-2,6-difluorophenyl]-2-
    ethoxyacetamide hydrochloride 701266-94-6P.
    N-(4-Carbamimidovlbenzvl)-2-ethoxy-2-(3-ethoxy-2.6-
    difluorophenyl)acetamide hydrochloride 701266-95-7P,
    N-(4-Carbamimidoylbenzyl)-2-(2,6-difluoro-3-propoxyphenyl)-2-
    ethoxyacetamide hydrochloride 701266-96-8P
, N-(4-Carbamimidovlbenzyl)-2-[3-(cyclopropylmethoxy)-2,6-difluorophenyl]-2-
    ethoxyacetamide hydrochloride 701266-97-9P.
    N-(4-Carbamimidoylbenzyl)-2-[3-(2-dimethylaminoethoxy)-2,6-difluorophenyl]-
    2-ethoxyacetamide dihydrochloride 701266-98-0P,
    N-(4-Carbamimidoylbenzyl)-2-[3-(cyclobutylmethoxy)-2,6-difluorophenyl]-2-
    ethoxyacetamide hydrochloride 701266-99-1P,
    N-(4-Carbamimidoylbenzyl)-2-[2,6-difluoro-3-[2-(2-oxopyrrolidin-1-
    yl)ethoxy]phenyl]-2-ethoxyacetamide hydrochloride 701267-00-7P,
    N-(4-Carbamimidoylbenzyl)-2-[2,6-difluoro-3-(3,3,3-
                                                               701267-01-8P,
    trifluoropropoxy)phenyl]-2-ethoxyacetamide hydrochloride
    N-(4-Carbamimidoylbenzyl)-2-[2,6-difluoro-3-[2-(pyridin-3-
    vl)ethoxv[phenvl]-2-ethoxvacetamide dihvdrochloride
                                                          701267-02-9P,
    N-(4-Carbamimidovlbenzvl)-2-[3-[(diethylcarbamovl)methoxvl-2,6-
    difluorophenvll-2-ethoxyacetamide hydrochloride 701267-03-0P.
    N-(4-Carbamimidovlbenzyl)-2-[2,6-difluoro-3-[2-(morpholin-4-
    yl)ethoxy]phenyl]-2-ethoxyacetamide dihydrochloride
                                                          701267-04-1P
                   701267-06-3P, N-(4-Carbamimidovlbenzyl)-2-[2,6-difluoro-3-
    701267-05-2P
    [2-(pyridin-2-yl)ethoxy]phenyl]-2-ethoxyacetamide dihydrochloride
    701267-07-4P 701267-08-5P, N-(4-Carbamimidoylbenzyl)-2-(2,6-difluoro-3-
    methoxyphenyl)-2-ethoxyacetamide hydrochloride
                                                    701267-09-6P.
    N-(4-Carbamimidoylbenzyl)-2-(3-cyclohexyloxy-2,6-difluorophenyl)-2-
    ethoxyacetamide hydrochloride 701267-10-9P,
    N-(4-Carbamimidoylbenzyl)-2-[2,6-difluoro-3-[(piperidin-4-yl)oxy]phenyl]-2-
    ethoxyacetamide dihydrochloride 701267-15-4P,
    N-(4-Carbamimidoylbenzyl)-2-[2,6-difluoro-3-(4-fluorophenoxy)phenyl]-2-
    ethoxyacetamide hydrochloride 701267-16-5P,
    N-(4-Carbamimidoylbenzyl)-2-[2,6-difluoro-3-[(pyridin-3-yl)oxy]phenyl]-2-
    ethoxyacetamide dihydrochloride
                                    701267-17-6P.
    N-(4-Carbamimidoylbenzyl)-2-[2,6-difluoro-3-[(3-
    trifluoromethylphenyl)oxylphenyl]-2-ethoxyacetamide hydrochloride
    701267-18-7P, N-(4-Carbamimidovlbenzvl)-2-[2,6-difluoro-3-(m-
    tolvloxy)phenv11-2-ethoxyacetamide hydrochloride
    N-(4-Carbamimidovlbenzyl)-2-ethoxy-2-[3-(3-ethoxyphenoxy)-2.6-
    difluorophenyllacetamide hydrochloride
                                            701267-23-4P.
    N-(4-Carbamimidoylbenzyl)-2-ethoxy-2-[3-(1-ethylpropoxy)-2,6-
    difluorophenyl]acetamide acetate
                                       701267-25-6P,
    N-(4-Carbamimidovlbenzyl)-2-(3-cyclopentyloxy-2,6-difluorophenyl)-2-
                              701267-27-8P,
    ethoxyacetamide acetate
    N-(4-Carbamimidovlbenzvl)-2-[2,6-difluoro-3-[(tetrahydropyran-4-
    vl)oxvlphenvll-2-ethoxvacetamide acetate
                                              701267-31-4P.
    N-(4-Carbamimidoylbenzyl)-2-[2,6-difluoro-3-(pyridin-2-yl)phenyl]-2-
    ethoxyacetamide dihydrochloride
                                      701267-32-5P,
    N-(4-Carbamimidoylbenzyl)-2-[2,6-difluoro-3-(6-methoxypyridin-3-yl)phenyl]-
    2-ethoxyacetamide dihydrochloride
                                        701267-33-6P,
    N-(4-Carbamimidoylbenzyl)-2-[2,6-difluoro-3-(pyridin-3-yl)phenyl]-2-
    ethoxyacetamide dihydrochloride
                                      701267-35-8P.
    N-(4-Carbamimidoylbenzyl)-2-[2,6-difluoro-3-(pyrimidin-5-yl)phenyl]-2-
    ethoxyacetamide dihydrochloride
                                      701267-36-9P,
    N-(4-Carbamimidoylbenzyl)-2-[2,6-difluoro-3-(pyridin-4-yl)phenyl]-2-
    ethoxyacetamide dihydrochloride
                                     701267-43-8P,
    N-(4-Carbamimidoylbenzyl)-2-(2,4-difluoro-3'-methylbiphenyl-3-yl)-2-
    methoxyacetamide 701267-44-9P, N-(4-Carbamimidoylbenzyl)-2-(2,4-difluoro-
    4'-methylbiphenyl-3-yl)-2-methoxyacetamide hydrochloride
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N-(4-Carbamimidoylbenzyl)-2-methoxy-2-(2,4,4'-trifluorobiphenyl-3-
vl)acetamide acetate
                     701267-47-2P,
N-(4-Carbamimidoylbenzyl)-2-(2,4-difluoro-4'-methylsulfanylbiphenyl-3-yl)-
2-methoxvacetamide hydrochloride 701267-49-4P,
N-(4-Carbamimidoylbenzyl)-2-(2,4-difluoro-3'-trifluoromethylbiphenyl-3-yl)-
                           701267-50-7P.
2-methoxyacetamide acetate
N-(4-Carbamimidoylbenzyl)-2-(2,4-difluoro-4'-methoxybiphenyl-3-vl)-2-
methoxyacetamide hydrochloride
                               701267-55-2P,
N-(4-Carbamimidovlbenzyl)-2-[2,6-difluoro-3-[(morpholin-4-
yl)carbonyl]phenyl]-2-methoxyacetamide acetate 701267-57-4P
701267-59-6P
              701267-61-0P 701267-63-2P 701267-65-4P
                                                          701267-66-5P,
N-(4-Carbamimidoylbenzyl)-2-[2,6-difluoro-3-[(pyridin-2-yl)methoxy]phenyl]-
2-methoxyacetamide dihydrochloride 701267-67-6P,
N-(4-Carbamimidoylbenzyl)-2-[2,6-difluoro-3-[(pyridin-3-yl)methoxy]phenyl]-
2-methoxyacetamide dihydrochloride 701267-68-7P,
N-(4-Carbamimidoylbenzyl)-2-[2,6-difluoro-3-[(pyridin-4-yl)methoxy]phenyl]-
2-methoxyacetamide dihydrochloride 701267-70-1P,
N-(4-Carbamimidoylbenzyl)-2-[2,6-difluoro-3-(4-fluorophenoxy)phenyl]-2-
methoxyacetamide acetate
                         701267-74-5P,
N-(4-Carbamimidoylbenzyl)-2-[2,6-difluoro-3-[(pyridin-3-yl)oxy]phenyl]-2-
methoxyacetamide acetate 701267-76-7P,
N-(4-Carbamimidovlbenzvl)-2-(3,5-difluorobiphenvl-4-vl)-2-methoxyacetamide
hvdrochloride
               701267-78-9P, N-(4-Carbamimidovlbenzvl)-2-(3,5-
difluorobiphenvl-4-vl)-2-ethoxyacetamide hydrochloride
                                                       701267-81-4P.
N-(4-Carbamimidoylbenzyl)-2-[2,6-difluoro-4-(1H-indol-5-yl)phenyl]-2-
                         701267-85-8P.
ethoxyacetamide acetate
N-(4-Carbamimidoylbenzyl)-2-[2,6-difluoro-4-(furan-2-yl)phenyl]-2-
ethoxyacetamide acetate 701267-87-0P,
N-(4-Carbamimidoylbenzyl)-2-[2,6-difluoro-4-(tetrahydrofuran-2-yl)phenyl]-
2-ethoxyacetamide acetate 701267-93-8P.
[[4'-[(4-Carbamimidoylbenzylcarbamoyl)(ethoxy)methyl]-3',5'-
difluorobiphenyl-3-yl]oxy]acetic acid 701267-95-0P,
N-(4-Carbamimidoylbenzyl)-2-[3'-(carbamoylmethoxy)-3,5-difluorobiphenyl-4-
v1]-2-ethoxyacetamide hydrochloride 701267-97-2P,
N-(4-Carbamimidoylbenzyl)-2-[3,5-difluoro-3'-(2-hydroxyethoxy)biphenyl-4-
vll-2-ethoxyacetamide hydrochloride 701267-99-4P,
N-(4-Carbamimidoylbenzyl)-2-[3'-(3-dimethylaminopropoxy)-3,5-
difluorobiphenyl-4-yl]-2-ethoxyacetamide hydrochloride
                                                        701268-05-5P.
2-[2'-(2-Benzyloxyethoxy)-3,5-difluorobiphenyl-4-yl]-N-(4-
carbamimidovlbenzvl)-2-ethoxyacetamide hydrochloride
                                                      701268-10-2P,
N-(4-Carbamimidoylbenzyl)-2-[2'-(2-dimethylaminoethoxy)-3,5-
difluorobiphenvl-4-vll-2-ethoxyacetamide hydrochloride
                                                       701268-12-4P.
N-(4-Carbamimidoylbenzyl)-2-[3,5-difluoro-2'-(2-hydroxyethoxy)biphenyl-4-
yl]-2-ethoxyacetamide hydrochloride
                                     701268-16-8P,
[[4'-[(4-Carbamimidoylbenzylcarbamoyl)(ethoxy)methyl]-3',5'-
difluorobiphenyl-2-yl]oxy]acetic acid 701268-21-5P,
N-(4-Carbamimidovlbenzyl)-2-[2'-(carbamovlmethoxy)-3,5-difluorobiphenyl-4-
                               701268-27-1P,
vll-2-ethoxvacetamide acetate
N-(4-Carbamimidoylbenzyl)-2-[2,6-difluoro-4-(pyridin-4-yl)phenyl]-2-
ethoxyacetamide hydrochloride 701268-29-3P,
N-(4-Carbamimidoylbenzyl)-2-[2,6-difluoro-4-(pyrimidin-5-yl)phenyl]-2-
ethoxyacetamide hydrochloride
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
(Uses)
   (anticoagulant; preparation of N-(carbamimidoylbenzyl)benzeneacetamides and
  pyridineacetamides as coagulation factor inhibitors)
701268-31-7P, N-(4-Carbamimidoylbenzyl)-2-[2,6-difluoro-4-(pyrimidin-2-
yl)phenyl]-2-ethoxyacetamide hydrochloride
                                            701268-33-9P,
N-(4-Carbamimidoylbenzyl)-2-[2,6-difluoro-4-(pyridin-2-yl)phenyl]-2-
ethoxyacetamide hydrochloride 701268-35-1P,
2-[4-(2-Aminopyrimidin-5-y1)-2,6-difluoropheny1]-N-(4-carbamimidoylbenzy1)-
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2-ethoxyacetamide hydrochloride
                                701268-38-4P.
N-(4-Carbamimidoylbenzyl)-2-[2,6-difluoro-4-(pyridin-3-yl)phenyl]-2-
                               701268-40-8P,
ethoxyacetamide hydrochloride
2-[4-(6-Aminopyridin-2-v1)-2,6-difluorophenv1]-N-(4-carbamimidovlbenzv1)-2-
ethoxyacetamide hydrochloride 701268-42-0P.
2-[4-(5-Aminopyridin-2-y1)-2,6-difluoropheny1]-N-(4-carbamimidoylbenzy1)-2-
ethoxyacetamide hydrochloride 701268-46-4P,
4'-[(4-Carbamimidoylbenzylcarbamoyl)(ethoxy)methyl]-3',5'-difluorobiphenyl-
3-carboxvlic acid 701268-50-0P, 2-[4-(6-Aminopyridin-3-v1)-2,6-
difluorophenvll-2-ethoxy-N-[4-(N-hydroxycarbamimidoyl)benzyllacetamide
701268-56-6P, N-(4-Carbamimidovlbenzvl)-2-(3,5-difluoro-2'-
hydroxymethylbiphenyl-4-yl)-2-ethoxyacetamide hydrochloride
701268-58-8P, N-(4-Carbamimidoylbenzyl)-2-(2'-chloromethyl-3,5-
difluorobiphenyl-4-yl)-2-ethoxyacetamide
                                          701268-61-3P,
2-(2'-Aminomethyl-3,5-difluorobiphenyl-4-yl)-N-(4-carbamimidoylbenzyl)-2-
                        701268-69-1P.
ethoxyacetamide acetate
N-(4-Carbamimidoylbenzyl)-2-(2-fluoro-4-methoxy-3-phenoxyphenyl)-2-
methoxyacetamide hydrochloride 701268-76-0P,
N-(4-Carbamimidoylbenzyl)-2-(2-ethyl-6-fluorophenyl)-2-methoxyacetamide
                701268-79-3P, N-(4-Carbamimidoylbenzyl)-2-[2-fluoro-6-(3-
hydrochloride
                                                       701268-81-7P,
hydroxypropyl)phenyl|-2-methoxyacetamide hydrochloride
N-(4-Carbamimidovlbenzvl)-2-(3-fluorobiphenvl-2-vl)-2-methoxvacetamide
              701268-82-8P, 2-(3'-Amino-3-fluorobiphenv1-2-v1)-N-(4-
carbamimidovlbenzvl)-2-methoxyacetamide hydrochloride
N-(4-Carbamimidoylbenzyl)-2-(3-fluoro-3'-nitrobiphenyl-2-yl)-2-
                                701268-85-1P.
methoxyacetamide hydrochloride
2-[2-(6-Aminopyridin-2-yl)-6-fluorophenyl]-N-(4-carbamimidoylbenzyl)-2-
methoxyacetamide acetate 701268-89-5P,
N-(4-Carbamimidovlbenzvl)-2-(2-fluoro-6-phenoxyphenyl)-2-methoxyacetamide
hydrochloride
              701268-90-8P, N-(4-Carbamimidoylbenzyl)-2-[2-(3-
dimethylaminopropoxy)-6-fluorophenyl]-2-methoxyacetamide hydrochloride
701268-91-9P, N-(4-Carbamimidoylbenzyl)-2-(2,6-difluoro-4-methoxyphenyl)-2-
ethoxyacetamide hydrochloride
                               701268-94-2P,
2-(4-Benzyloxy-2,6-difluorophenyl)-N-(4-carbamimidoylbenzyl)-2-
ethoxyacetamide hydrochloride
                               701268-99-7P,
N-(4-Carbamimidoylbenzyl)-2-(2,6-difluoro-4-isopropoxyphenyl)-2-
ethoxyacetamide hydrochloride 701269-01-4P,
N-(4-Carbamimidoylbenzyl)-2-[2,6-difluoro-4-[(pyridin-2-yl)methoxy]phenyl]-
2-ethoxyacetamide hydrochloride
                                 701269-05-8P,
2-[2,6-Difluoro-4-(pyridin-2-vlmethoxy)phenyl]-2-ethoxy-N-[4-(N-
hvdroxvcarbamimidovl)benzvllacetamide
                                       701269-07-0P,
[Amino[4-[[[2-[2,6-difluoro-4-(pyridin-2-vlmethoxy)phenyl]-2-
ethoxyacetyl]amino]methyl]phenyl]methylene]carbamic acid ethyl ester
701269-08-1P, N-(4-Carbamimidoylbenzyl)-2-[2,6-difluoro-4-[(pyridin-3-
yl)methoxy[phenyl]-2-ethoxyacetamide hydrochloride
                                                    701269-09-2P,
N-(4-Carbamimidovlbenzyl)-2-[2,6-difluoro-4-[(pyridin-4-yl)methoxy|phenyl]-
                                 701269-11-6P,
2-ethoxyacetamide hydrochloride
N-(4-Carbamimidoylbenzyl)-2-(2,6-difluoro-4-phenoxyphenyl)-2-
ethoxyacetamide hydrochloride
                               701269-12-7P.
N-(4-Carbamimidoylbenzyl)-2-[2,6-difluoro-4-[(pyridin-3-yl)oxy]phenyl]-2-
                               701269-13-8P,
ethoxyacetamide hydrochloride
N-(4-Carbamimidovlbenzyl)-2-(2,6-difluoro-3-isopropoxyphenyl)-2-
ethoxyacetamide hydrochloride
                               701269-14-9P,
N-(4-Carbamimidovlbenzvl)-2-[3-(carbamovlmethoxv)-2,6-difluorophenvl]-2-
                               701269-15-0P,
ethoxyacetamide hydrochloride
2-[3-(2-Benzyloxyethoxy)-2,6-difluorophenyl]-N-(4-carbamimidoylbenzyl)-2-
ethoxyacetamide hydrochloride
                               701269-16-1P,
N-(4-Carbamimidoylbenzyl)-2-[2,6-difluoro-3-(2-hydroxyethoxy)phenyl]-2-
ethoxyacetamide hydrochloride 701269-19-4P,
N-(4-Carbamimidoylbenzyl)-2-(2,6-difluoro-3-phenoxyphenyl)-2-
ethoxyacetamide acetate 701269-20-7P,
N-(4-Carbamimidoylbenzyl)-2-(2,4-difluorobiphenyl-3-yl)-2-ethoxyacetamide
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hydrochloride
              701269-29-6P, N-(4-Carbamimidoylbenzyl)-2-(2,6-difluoro-3-
phenylaminophenyl)-2-methoxyacetamide acetate
                                               701269-32-1P,
N-(4-Carbamimidoylbenzyl)-2-(2,6-difluoro-3-isopropylaminophenyl)-2-
                         701269-33-2P.
methoxvacetamide acetate
2-(3-Acetylamino-2,6-difluorophenyl)-N-(4-carbamimidoylbenzyl)-2-
methoxyacetamide hydrochloride
                               701269-34-3P.
N-(4-Carbamimidoylbenzyl)-2-[2,6-difluoro-3-[(phenylacetyl)amino]phenyl]-2-
methoxyacetamide hydrochloride 701269-39-8P,
N-(4-Carbamimidovlbenzvl)-2-(2,6-difluoro-3-hydroxymethylphenyl)-2-
ethoxyacetamide hydrochloride 701269-44-5P,
2-[3-[(Acetylamino)methyl]-2,6-difluorophenyl]-N-(4-carbamimidoylbenzyl)-2-
ethoxyacetamide hydrochloride 701269-47-8P.
2-(3-Aminomethyl-2,6-difluorophenyl)-N-(4-carbamimidoylbenzyl)-2-
ethoxyacetamide acetate 701269-49-0P,
N-(4-Carbamimidoylbenzyl)-2-[2,6-difluoro-3-[(phenylamino)methyl]phenyl]-2-
ethoxyacetamide hydrochloride 701269-50-3P,
N-(4-Carbamimidoylbenzyl)-2-[2,6-difluoro-3-[(morpholin-4-
yl)methyl]phenyl]-2-ethoxyacetamide hydrochloride
                                                  701269-51-4P.
N-(4-Carbamimidoylbenzyl)-2-[2,6-difluoro-3-[(piperidin-1-
yl)methyl]phenyl]-2-ethoxyacetamide hydrochloride 701269-54-7P,
N-(4-Carbamimidoylbenzyl)-2-(2,6-difluoro-3-formylphenyl)-2-
ethoxvacetamide acetate
                        701269-57-0P,
N-(4-Carbamimidov1-2,6-difluorobenzv1)-2-(2,6-difluoro-4-methoxyphenv1)-2-
ethoxyacetamide hydrochloride 701269-59-2P.
N-(4-Carbamimidoy1-2,6-difluorobenzy1)-2-ethoxy-2-(2-fluoro-4-
methoxyphenyl)acetamide acetate
                                701269-61-6P,
N-(4-Carbamimidoy1-2,6-difluorobenzy1)-2-(2,6-difluoro-4-methoxypheny1)-2-
methoxyacetamide acetate 701269-63-8P,
N-(4-Carbamimidov1-2,6-difluorobenzv1)-2-(2-fluoro-4-methoxyphenv1)-2-
methoxyacetamide acetate 701269-69-4P.
N-[4-Carbamimidoy1-2-[(carbamoy1methy1)amino]benzy1]-2-ethoxv-2-(2-fluoro-
4-methoxyphenyl)acetamide hydrochloride 701269-71-8P,
N-(2-Benzylamino-4-carbamimidoylbenzyl)-2-ethoxy-2-(2-fluoro-4-
methoxyphenyl)acetamide acetate
                                701269-72-9P,
N-[4-Carbamimidov1-2-(2-fluorobenzylamino)benzyl]-2-ethoxy-2-(2-fluoro-4-
methoxyphenyl)acetamide hydrochloride
                                      701269-73-0P.
N-[4-Carbamimidoy1-2-[(pyridin-2-ylmethy1)amino]benzy1]-2-ethoxy-2-(2-
fluoro-4-methoxyphenyl)acetamide hydrochloride
                                                701269-74-1P,
N-[4-Carbamimidoy1-2-(4-chloro-2-fluorobenzylamino)benzyl]-2-ethoxy-2-(2-
fluoro-4-methoxyphenyl)acetamide hydrochloride 701269-75-2P,
N-(4-Carbamimidov1-2-phenethylaminobenzyl)-2-ethoxy-2-(2-fluoro-4-
methoxyphenyl)acetamide hydrochloride
                                       701269-78-5P.
[[5-Carbamimidoy1-2-[[[2-ethoxy-2-(2-fluoro-4-
methoxyphenyl)acetyl]amino]methyl]phenyl]amino]acetic acid acetate
701269-80-9P, N-[4-Carbamimidoy1-2-[(phenylmethylsulfonyl)amino]benzyl]-2-
ethoxy-2-(2-fluoro-4-methoxyphenyl)acetamide hydrochloride
                                                           701269-82-1P,
N-[2-(3-Benzylureido)-4-carbamimidoylbenzyl]-2-ethoxy-2-(2-fluoro-4-
                                701269-83-2P,
methoxyphenyl)acetamide acetate
[5-Carbamimidoy1-2-[[[2-ethoxy-2-(2-fluoro-4-
methoxyphenyl)acetyl]amino]methyl]phenyl]carbamic acid benzyl ester
               701269-85-4P, N-(4-Carbamimidoy1-2-phenylaminobenzy1)-2-
hydrochloride
ethoxy-2-(2-fluoro-4-methoxyphenyl)acetamide hydrochloride
                                                           701269-89-8P,
2-[4-(6-Aminopyridin-3-v1)-2,6-difluorophenv1]-N-[4-carbamimidov1-2-
(carbamoylmethoxy)benzyl]-2-ethoxyacetamide hydrochloride
                                                           701269-92-3P.
N-[4-Carbamimidoyl-2-(carbamoylmethoxy)benzyl]-2-[2,6-difluoro-4-[(pyridin-
2-y1)methoxy]pheny1]-2-ethoxyacetamide hydrochloride 701269-96-7P,
2-[4-(6-Aminopyridin-3-yl)-2,6-difluorophenyl]-N-(4-carbamimidoyl-2,6-
difluorobenzy1)-2-ethoxyacetamide acetate
                                          701270-01-1P,
(S)-N-(4-Carbamimidoy1benzy1)-2-(2,6-difluoro-4-methoxypheny1)-2-
methoxyethanamide formate 701270-04-4P 701270-09-9P,
(R)-N-(4-Carbamimidoylbenzyl)-2-ethoxy-2-(2-fluoro-4-
methoxyphenyl)ethanamide acetate 701270-10-2P,
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[Amino[4-[[[2-ethoxy-2-(2-fluoro-4-
methoxyphenyl)acetyl|amino|methyl|phenyl|methylene|carbamic acid benzyl
        701270-11-3P, [[4-[[[2-(2,6-Difluoro-4-methoxypheny1)-2-
methoxyacetyllamino|methyl|phenyl|(imino)methyl|carbamic acid benzyl ester
701270-18-0P, N-(4-Carbamimidoylbenzyl)-2-[2,6-difluoro-4-(1-oxopyridin-4-
                                             701270-21-5P.
yl)phenyl]-2-methoxyacetamide hydrochloride
N-(4-Carbamimidoylbenzyl)-2-[2,6-difluoro-4-(tetrahydropyran-4-yl)phenyl]-
2-ethoxyacetamide acetate
                           701270-23-7P,
N-(4-Carbamimidovlbenzvl)-2-(4-cvclohexvl-2,6-difluorophenvl)-2-
ethoxyacetamide acetate
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
(Uses)
   (anticoagulant; preparation of N-(carbamimidoylbenzyl)benzeneacetamides and
   pyridineacetamides as coagulation factor inhibitors)
701263-56-1P, N-(4-Carbamimidoylbenzyl)-2-(2-fluoro-4-methoxyphenyl)-2-
methoxyacetamide hydrochloride 701263-57-2P,
[Amino[4-[[2-(2-fluoro-4-methoxyphenyl)-2-
methoxyacetyl]amino]methyl]phenyl]methylene]carbamic acid ethyl ester
701263-58-3P, 2-(2-Fluoro-4-methoxyphenyl)-N-(4-(N-
hvdroxvcarbamimidovl)benzvl]-2-methoxvacetamide
                                                 701264-58-6P,
N-(4-Carbamimidovlbenzvl)-2-ethoxv-2-(2-fluoro-4-methoxyphenvl)acetamide
hydrochloride
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic
preparation); THU (Therapeutic use); BIOL (Biological study); PREP
(Preparation); RACT (Reactant or reagent); USES (Uses)
   (intermediate, anticoagulant; preparation of
   N-(carbamimidovlbenzvl)benzeneacetamides and pyridineacetamides as
   coagulation factor inhibitors)
701272-58-4P
RL: PEP (Physical, engineering or chemical process); PYP (Physical
process); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)
   (intermediate; preparation of N-(carbamimidoylbenzyl)benzeneacetamides and
   pyridineacetamides as coagulation factor inhibitors)
701270-06-6P, (R)-Ethoxy(2-fluoro-4-methoxyphenyl)ethanoic acid ethyl
ester
       701272-60-8P
                      701272-62-0P
RL: PUR (Purification or recovery); RCT (Reactant); SPN (Synthetic
preparation); PREP (Preparation); RACT (Reactant or reagent)
   (intermediate; preparation of N-(carbamimidoylbenzyl)benzeneacetamides and
   pyridineacetamides as coagulation factor inhibitors)
7472-67-5P, 2-Methoxy-2-phenylpropionic acid
(2-Chlorophenyl) (methoxy) acetic acid
                                      42164-79-4P.
Hydroxy(3-nitrophenyl)acetic acid
                                  59769-10-7P.
2-Methoxy-2-(pyridin-2-yl)acetic acid 90178-72-6P,
4-Formy1-3-phenoxybenzonitrile
                                90536-45-1P,
(4-Hydroxyphenyl) (methoxy) acetic acid
                                       91004-43-2P,
Methoxy(3-nitrophenyl)acetic acid
                                  93555-01-2P,
(3-Nitrophenyl)trimethylsilanyloxyacetonitrile
                                                103441-02-7P,
                                     200571-27-3P.
(2-Fluorophenyl) (methoxy) acetic acid
Methoxy(3-nitrophenyl)acetic acid methyl ester 207454-14-6P,
                                             504414-32-8P,
(4-Dimethylaminophenyl) (methoxy) acetic acid
4-Benzyloxy-2-fluorobenzaldehyde
                                  537013-51-7P,
4-Bromo-2,6-difluorobenzaldehyde
                                   701263-27-6P,
(S)=N-(4-Cyanobenzyl)-α-methoxybenzeneethanamide
                                                  701263-29-8P.
(R) -N-(4-Cyanobenzyl)-α-methoxybenzeneethanamide 701263-32-3P,
(4-Benzyloxyphenyl) (methoxy) acetic acid 701263-33-4P,
2-(4-Benzyloxyphenyl)-N-(4-cyanobenzyl)-2-methoxyacetamide 701263-35-6P,
Methoxy(4-phenoxyphenyl)acetic acid
                                     701263-36-7P,
N-(4-Cyanobenzy1)-2-methoxy-2-(4-phenoxypheny1)acetamide
                                                           701263-38-9P,
N-(4-Cyanobenzyl)-2-methoxy-2-(3-phenoxyphenyl)acetamide
                                                           701263-40-3P
701263-42-5P, N-(4-Cyanobenzyl)-2-(2-fluorophenyl)-2-methoxyacetamide
701263-51-6P, [5-Ethoxy-2-fluoro-3-(1-methylpiperidin-4-
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yloxy)phenyl] (methoxy)acetic acid 701263-52-7P,
N-(4-Cyanobenzyl)-2-[5-ethoxy-2-fluoro-3-[(1-methylpiperidin-4-
y1)oxy]pheny1]-2-methoxyacetamide 701263-54-9P,
(2-Fluoro-4-methoxyphenyl) (methoxy) acetic acid 701263-55-0P,
N-(4-Cvanobenzv1)-2-(2-fluoro-4-methoxyphenv1)-2-methoxyacetamide
701263-60-7P, (3-Hydroxy-4-methoxyphenyl) (methoxy) acetic acid
701263-61-8P, [5-[(4-Cyanobenzylcarbamoyl)(methoxy)methyl]-2-
methoxyphenoxy|acetic acid ethyl ester
                                        701263-64-1P,
Ethoxy(3-hydroxy-4-methoxyphenyl)acetic acid
                                             701263-65-2P,
[5-[(4-Cvanobenzylcarbamovl)(ethoxy)methyl]-2-methoxyphenoxylacetic acid
ethvl ester
            701263-69-6P, N-(4-Cvanobenzyl)-2-(4-hydroxyphenyl)-2-
methoxyacetamide
                  701263-70-9P, N-(4-Cyanobenzyl)-2-(4-ethoxyphenyl)-2-
methoxyacetamide
                  701263-72-1P, N-(4-Cyanobenzyl)-2-methoxy-2-[4-[(1-
methylpiperidin-4-vl)oxv|phenyl|acetamide
                                          701263-75-4P,
(2-Fluoro-4,5-dimethoxyphenyl) (methoxy) acetic acid
                                                   701263-76-5P,
N-(4-Cyanobenzyl)-2-(2-fluoro-4,5-dimethoxyphenyl)-2-methoxyacetamide
701263-79-8P, N-(4-Cyanobenzyl)-2-(3-isopropoxyphenyl)-2-methoxyacetamide
701263-83-4P, N-(4-Cyanobenzyl)-2-(4-isopropoxyphenyl)-2-methoxyacetamide
701263-85-6P, [4-[(4-Cyanobenzylcarbamoyl)(methoxy)methyl]phenoxy]acetic
acid ethyl ester
                 701263-90-3P, (3,5-Diethoxy-2-
                                   701263-91-4P,
fluorophenvl) (methoxy) acetic acid
N-(4-Cvanobenzvl)-2-(3,5-diethoxy-2-fluorophenyl)-2-methoxyacetamide
701263-93-6P, [5-Ethoxy-2-fluoro-4-(2-hydroxyethoxy)phenyl] (methoxy)acetic
      701263-94-7P, N-(4-Cyanobenzyl)-2-15-ethoxy-2-fluoro-4-(2-
hydroxyethoxy)phenyl]-2-methoxyacetamide 701263-97-0P,
(3,4-Diethoxy-2-fluorophenyl) (methoxy) acetic acid
                                                  701263-98-1P.
N-(4-Cyanobenzyl)-2-(3,4-diethoxy-2-fluorophenyl)-2-methoxyacetamide
701264-00-8P, 4-Aminomethyl-3-fluorobenzonitrile 701264-01-9P,
N-(4-Cvano-2-fluorobenzyl)-2-(2-fluoro-4-methoxyphenyl)-2-methoxyacetamide
701264-03-1P, N-(4-Cyano-3-fluorobenzyl)-2-(2-fluoro-4-methoxyphenyl)-2-
methoxyacetamide 701264-06-4P, (2-Benzyloxy-4-
methoxyphenyl) (methoxy) acetic acid
                                   701264-07-5P,
(2-Hydroxy-4-methoxyphenyl) (methoxy) acetic acid 701264-08-6P,
N-(4-Cyanobenzyl)-2-(2-hydroxy-4-methoxyphenyl)-2-methoxyacetamide
701264-09-7P, N-[4-(N-Hydroxycarbamimidoyl)benzyl]-2-(2-hydroxy-4-
methoxyphenyl)-2-methoxyacetamide 701264-16-6P,
2-(4-Bromo-2-fluorophenyl)-N-(4-cyanobenzyl)-2-ethoxyacetamide
701264-18-8P, 2-(4-Bromo-2-fluorophenyl)-N-(4-cyanobenzyl)-2-
propoxyacetamide
                 701264-21-3P, N-(4-Cyanobenzyl)-2-[4-(2-
hydroxyethoxy)phenyl]-2-methoxyacetamide
                                         701264-23-5P,
N-(4-Cvanobenzvl)-2-(4-dimethylaminophenyl)-2-methoxyacetamide
701264-26-8P, N-(4-Cvanobenzyl)-2-methoxy-2-[4-(pyrrolidin-1-
vl)phenvllacetamide
                     701264-28-0P.
2-(2-Chlorophenyl)-N-(4-cyanobenzyl)-2-methoxyacetamide
                                                        701264-30-4P,
(4-Acetylaminophenyl) (methoxy) acetic acid
                                          701264-31-5P,
2-(4-Acetylaminophenyl)-N-(4-cyanobenzyl)-2-methoxyacetamide
701264-33-7P, Methoxy(4-trifluoromethoxyphenyl)acetic acid
                                                            701264-34-8P.
N-(4-Cvanobenzvl)-2-methoxv-2-(4-trifluoromethoxyphenvl)acetamide
701264-36-0P, N-(4-Cyanobenzyl)-2-[4-(imidazol-1-yl)phenyl]-2-
methoxyacetamide 701264-38-2P, Methoxy(6-methoxynaphthalen-2-yl)acetic
      701264-39-3P, N-(4-Cyanobenzyl)-2-methoxy-2-(6-methoxynaphthalen-2-
vl)acetamide
              701264-41-7P, N-(4-Cyanobenzyl)-2-methoxy-2-[4-(morpholin-4-
vl)phenvl|acetamide 701264-44-0P,
N-(4-Cyanobenzyl)-2-[4-(3-dimethylaminopropoxy)phenyl]-2-methoxyacetamide
701264-47-3P, N-(4-Cyanobenzyl)-2-(4'-dimethylamino-3-fluorobiphenyl-4-yl)-
2-methoxyacetamide
                    701264-53-1P,
(2,2-Dimethylchroman-6-yl) (methoxy) acetic acid 701264-54-2P,
N-(4-Cyanobenzy1)-2-(2,2-dimethylchroman-6-y1)-2-methoxyacetamide
701264-56-4P, Ethoxy(2-fluoro-4-methoxyphenyl)acetic acid
                                                           701264-57-5P,
N-(4-Cyanobenzyl)-2-ethoxy-2-(2-fluoro-4-methoxyphenyl)acetamide
701264-60-0P, (3-Cyclopentyloxy-4-methoxyphenyl) (methoxy) acetic acid
701264-62-2P, (2-Chloro-4-methoxyphenyl) (methoxy) acetic acid
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701264-63-3P, 2-(2-Chloro-4-methoxyphenyl)-N-(4-cyanobenzyl)-2-
                  701264-65-5P, (2,6-Difluoro-4-
methoxyacetamide
methoxyphenyl) (methoxy) acetic acid 701264-66-6P,
N-(4-Cyanobenzyl)-2-(2,6-difluoro-4-methoxyphenyl)-2-methoxyacetamide
701264-68-8P, N-(4-Cyanobenzy1)-2-(2-fluoro-4-methoxypheny1)-2-
propoxyacetamide 701264-70-2P, N-(4-Cyanobenzyl)-2-methoxy-2-(naphthalen-
1-yl)propionamide 701264-72-4P, 2-(4-Bromo-2,6-difluorophenyl)-N-(4-
cyanobenzyl)-2-methoxyacetamide 701264-74-6P,
(4-Benzyloxy-2-fluorophenyl) (methoxy) acetic acid
                                                  701264-75-7P,
(2-Fluoro-4-hydroxyphenyl) (methoxy) acetic acid 701264-76-8P,
N-(4-Cvanobenzyl)-2-(2-fluoro-4-hydroxyphenyl)-2-methoxyacetamide
701264-77-9P, N-(4-Cyanobenzy1)-2-(2-fluoro-4-isopropoxypheny1)-2-
methoxyacetamide 701264-79-1P, N-(4-Cyanobenzyl)-2-(2-fluoro-4-
isobutoxyphenyl)-2-methoxyacetamide 701264-81-5P,
N-(4-Cyanobenzyl)-2-[2-fluoro-4-[2-(4-fluorophenyl)ethoxy]phenyl]-2-
                 701264-83-7P, N-(4-Cyanobenzyl)-2-[2-fluoro-4-(4,4,5,5-
methoxvacetamide
tetramethyl-[1,3,2]dioxaborolan-2-yl)phenyl]-2-methoxyacetamide
701264-84-8P, N-(4-Cyanobenzyl)-2-[2-fluoro-4-(pyridin-3-yl)phenyl]-2-
methoxyacetamide 701264-86-0P, N-(4-Cyanobenzyl)-2-[2-fluoro-4-(pyridin-
4-v1)phenyl]-2-methoxyacetamide
                                701264-88-2P,
(5-Bromo-2-fluorophenvl) (methoxy) acetic acid
                                              701264-89-3P,
2-(5-Bromo-2-fluorophenyl)-N-(4-cyanobenzyl)-2-methoxyacetamide
701264-91-7P, N-(4-Cvanobenzvl)-2-(4-fluorobiphenvl-3-vl)-2-
                 701264-93-9P, (2-Fluoro-5-methylphenyl) (methoxy) acetic
methoxyacetamide
      701264-94-0P, N-(4-Cyanobenzyl)-2-(2-fluoro-5-methylphenyl)-2-
methoxyacetamide 701264-96-2P, (2-Fluoro-5-
                                           701264-97-3P.
trifluoromethylphenyl) (methoxy) acetic acid
N-(4-Cyanobenzyl)-2-(2-fluoro-5-trifluoromethylphenyl)-2-methoxyacetamide
701264-99-5P, (2-Fluoro-6-methoxyphenyl) (methoxy) acetic acid
701265-00-1P, N-(4-Cyanobenzyl)-2-(2-fluoro-6-methoxyphenyl)-2-
methoxyacetamide 701265-03-4P, 2-Benzyloxy-6-fluorobenzaldehyde
701265-04-5P, (2-Benzyloxy-6-fluorophenyl) (methoxy) acetic acid
701265-05-6P, (2-Fluoro-6-hydroxyphenyl) (methoxy) acetic acid
701265-06-7P, N-(4-Cyanobenzyl)-2-(2-fluoro-6-hydroxyphenyl)-2-
                  701265-07-8P 701265-08-9P
methoxvacetamide
                                                701265-10-3P
701265-12-5P 701265-14-7P 701265-16-9P 701265-18-1P,
[(4-Cyanobenzylcarbamoyl)phenylmethyl]carbamic acid tert-butyl ester
701265-20-5P 701265-21-6P 701265-22-7P,
N-(4-Cyanobenzyl)-2-[2-fluoro-4-(2-phenoxyethoxy)phenyl]-2-
methoxyacetamide 701265-24-9P, N-(4-Cvanobenzyl)-2-methoxy-2-(pyridin-2-
vl)acetamide
             701265-26-1P, N-(4-Cvanobenzvl)-2-methoxv-2-
phenylpropionamide 701265-29-4P.
N-(4-Cyanobenzyl)-2-[2-fluoro-6-(2-hydroxyethoxy)phenyl]-2-
methoxyacetamide 701265-31-8P, 2-[2-(Carbamoylmethoxy)-6-fluorophenyl]-N-
(4-cyanobenzyl)-2-methoxyacetamide
                                   701265-33-0P,
2-(Biphenvl-4-vl)-2-ethoxypropionic acid ethyl ester
                                                     701265-34-1P.
2-(Biphenyl-4-yl)-2-ethoxypropionic acid 701265-35-2P,
2-(Biphenyl-4-yl)-N-(4-cyanobenzyl)-2-ethoxypropionamide
                                                         701265-38-5P,
4-[3-[(Carboxymethoxy)methyl]-5-ethoxy-2-fluorophenoxy]piperidine-1-
carboxylic acid tert-butyl ester 701265-39-6P,
4-[3-[(4-Cyanobenzylcarbamoyl)(methoxy)methyl]-5-ethoxy-2-
fluorophenoxy]piperidine-1-carboxylic acid tert-butyl ester
701265-40-9P, N-(4-Cvanobenzyl)-2-[5-ethoxy-2-fluoro-3-[(piperidin-4-
yl)oxy]phenyl]-2-methoxyacetamide
                                  701265-41-0P.
2-[3-[1-(Benzenesulfonyl)piperidin-4-yloxy]-5-ethoxy-2-fluorophenyl]-N-(4-
cyanobenzyl)-2-methoxyacetamide 701265-46-5P,
N-(2-Chloro-4-cyanobenzyl)-2-(2-fluoro-4-methoxyphenyl)-2-methoxyacetamide
701265-48-7P, N-(2-Chloro-4-cyanobenzyl)-2-ethoxy-2-(2-fluoro-4-
methoxyphenyl)acetamide
                        701265-50-1P,
(2,6-Difluoro-4-methoxyphenyl)(hydroxy)acetic acid ethyl ester
701265-51-2P, (2,6-Difluoro-4-methoxyphenyl)(ethoxy)acetic acid ethyl
ester 701265-52-3P, (2,6-Difluoro-4-methoxyphenyl)(ethoxy)acetic acid
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701265-53-4P, N-(2-Chloro-4-cyanobenzyl)-2-(2,6-difluoro-4-methoxyphenyl)-
2-ethoxyacetamide
                   701265-55-6P, N-(2-Chloro-4-cyanobenzyl)-2-(2,6-
difluoro-4-methoxyphenyl)-2-methoxyacetamide
                                              701265-57-8P,
N-(3-Chloro-4-cvanobenzyl)-2-ethoxy-2-(2-fluoro-4-methoxyphenyl)acetamide
701265-58-9P, N-13-Chloro-4-(N-hydroxycarbamimidoyl)benzyl]-2-ethoxy-2-(2-
fluoro-4-methoxyphenyl)acetamide
                                  701265-62-5P.
N-(4-Cyano-2-methoxybenzyl)-2-ethoxy-2-(2-fluoro-4-methoxyphenyl)acetamide
701265-64-7P, 4-[(Hydroxyimino)methyl]-3-phenoxybenzonitrile
              701265-66-9P, N-(4-Cvano-2-phenoxybenzyl)-2-ethoxy-2-(2-
701265-65-8P
                                 701265-72-7P,
fluoro-4-methoxyphenyl)acetamide
3-Hydroxy-4-[(hydroxyimino)methyl]benzonitrile
                                                701265-73-8P.
4-Aminomethyl-3-hydroxybenzonitrile hydrochloride 701265-74-9P,
N-(4-Cyano-2-hydroxybenzyl)-2-ethoxy-2-(2-fluoro-4-methoxyphenyl)acetamide
701265-75-0P, N-[4-Cyano-2-(5-nitropyridin-2-yloxy)benzyl]-2-ethoxy-2-(2-
fluoro-4-methoxyphenyl)acetamide 701265-78-3P 701265-79-4P,
N-(5-Cyanobiphenyl-2-ylmethyl)-2-ethoxy-2-(2-fluoro-4-
methoxyphenyl)acetamide 701265-81-8P,
[5-Cyano-2-[[[2-ethoxy-2-(2-fluoro-4-
methoxyphenyl)acetyl]amino]methyl]phenoxy]acetic acid ethyl ester
701265-92-1P, [2-(Carbamoylmethoxy)-4-cyanobenzyl]carbamic acid tert-butyl
       701265-93-2P, 2-(2-Aminomethyl-5-cvanophenoxy)acetamide
hydrochloride
               701265-95-4P, N-(4-Cyano-2-phenoxybenzyl)-2-(2,6-difluoro-
                                    701265-97-6P,
4-methoxyphenyl)-2-ethoxyacetamide
4-[[3-(2,6-Difluoro-4-methoxyphenyl]-3-ethoxy-2-oxopropyl]amino]-3-
methoxybenzonitrile
                    701265-99-8P,
N-(4-Cyano-2-hydroxybenzyl)-2-(2,6-difluoro-4-methoxyphenyl)-2-
ethoxyacetamide 701266-00-4P, N-[2-(Carbamoylmethoxy)-4-cyanobenzyl]-2-
(2,6-difluoro-4-methoxyphenyl)-2-ethoxyacetamide
                                                  701266-10-6P
701266-12-8P 701266-15-1P, N-(4-Cyano-2-hydroxybenzyl)-2-(2,6-difluoro-4-
methoxyphenyl)-2-methoxyacetamide
                                   701266-16-2P.
N-[4-Cyano-2-[(methylcarbamoyl)methoxy]benzyl]-2-(2,6-difluoro-4-
methoxyphenyl)-2-methoxyacetamide 701266-21-9P,
N-[4-Cyano-2-(2,2,2-trifluoroethoxy)benzyl]-2-(2,6-difluoro-4-
methoxyphenyl)-2-methoxyacetamide
                                   701266-25-3P,
                                               701266-26-4P.
tert-Butyl(3,5-difluorophenoxy)diphenylsilane
[4-(tert-Butyldiphenylsilanyloxy)-2,6-difluorophenyl](hydroxy)acetic acid
ethvl ester
             701266-27-5P, [4-(tert-Butyldiphenylsilanyloxy)-2,6-
difluorophenyl](ethoxy)acetic acid ethyl ester
                                                701266-28-6P,
(2,6-Difluoro-4-hydroxyphenyl) (ethoxy) acetic acid
                                                   701266-29-7P,
[[4-[[[2-(2,6-Difluoro-4-hydroxyphenyl]-2-
ethoxyacetyllamino|methyl|phenyl|(imino)methyl|carbamic acid benzyl ester
701266-30-0P, (2.6-Difluoro-4-hydroxyphenyl)(ethoxy)acetic acid ethyl
       701266-32-2P, [[4-[[[2-[2,6-Difluoro-4-[2-(morpholin-4-
yl)ethoxy[phenyl]-2-ethoxyacetyl]amino]methyl]phenyl](imino)methyl]carbami
c acid benzyl ester
                     701266-37-7P,
[2,6-Difluoro-4-(4-methoxyphenoxy)phenyl](ethoxy)acetic acid ethyl ester
701266-38-8P, [2,6-Difluoro-4-(4-methoxyphenoxy)phenyl] (ethoxy)acetic acid
701266-39-9P, [[4-[[[2-[2,6-Difluoro-4-(4-methoxyphenoxy)phenyl]-2-
ethoxyacetyl]amino]methyl]phenyl](imino)methyl]carbamic acid benzyl ester
701266-41-3P, [4-(3,4-Dimethoxyphenoxy)-2,6-difluorophenyl](ethoxy)acetic
       701266-42-4P, [[4-[[[2-[4-(3,4-Dimethoxyphenoxy)-2,6-
difluorophenyl]-2-ethoxyacetyl]amino]methyl]phenyl](imino)methyl]carbamic
acid benzvl ester
                   701266-44-6P,
[2,6-Difluoro-4-(3-methoxyphenoxy)phenyl] (ethoxy)acetic acid ethyl ester
701266-45-7P, [2,6-Difluoro-4-(3-methoxyphenoxy)phenyl] (ethoxy)acetic acid
701266-46-8P, [[4-[[2-[2,6-Difluoro-4-(3-methoxyphenoxy)pheny1]-2-
ethoxyacetyl]amino]methyl]phenyl](imino)methyl]carbamic acid benzyl ester
701266-48-0P, [4-(3-Acetylaminophenoxy)-2,6-difluorophenyl](ethoxy)acetic
acid ethyl ester
                  701266-49-1P, [4-(3-Acetylaminophenoxy)-2,6-
difluorophenyl] (ethoxy) acetic acid
                                   701266-50-4P.
[[4-[[[2-[4-(3-Acetylaminophenoxy)-2,6-difluorophenyl]-2-
ethoxyacetyl]amino]methyl]phenyl](imino)methyl]carbamic acid benzyl ester
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701266-52-6P, [4-(4-Cyanophenoxy)-2,6-difluorophenyl](ethoxy)acetic acid
701266-53-7P, [[4-[[2-[4-(4-Cyanophenoxy)-2,6-difluoropheny1]-2-
ethoxyacetyl|amino|methyl|phenyl|(imino)methyl|carbamic acid benzyl ester
701266-55-9P, [2,6-Difluoro-4-(3-
trifluoromethoxyphenoxy)phenyll(ethoxy)acetic acid ethyl ester
701266-56-0P, [2,6-Difluoro-4-(3-
trifluoromethoxyphenoxy)phenyl](ethoxy)acetic acid
                                                   701266-57-1P.
[[4-[[[2-[2,6-Difluoro-4-(3-trifluoromethoxyphenoxy)phenyl]-2-
ethoxyacetyllamino|methyl|phenyl|(imino)methyl|carbamic acid benzyl ester
701266-59-3P, [2,6-Difluoro-4-
[(trifluoromethanesulfonyl)oxy]phenyl](ethoxy)acetic acid ethyl ester
701266-60-6P, 4-[(2-Ethoxyethoxycarbonyl)methyl]-3,5-difluorobenzoic acid
2-(trimethylsilanyl)ethyl ester 701266-61-7P,
4-[(2-Ethoxyethoxycarbonyl)methyl]-3,5-difluorobenzoic acid
701266-62-8P, [2,6-Difluoro-4-(isobutylcarbamoyl)phenyl](ethoxy)acetic
                 701266-63-9P, [2,6-Difluoro-4-
acid ethvl ester
(isobutylcarbamoyl)phenyl](ethoxy)acetic acid
[[4-[[[2-[2,6-Difluoro-4-(isobutylcarbamoyl)phenyl]-2-
ethoxyacetyl]amino]methyl]phenyl](imino)methyl]carbamic acid benzyl ester
701266-71-9P, tert-Butyl(2,4-difluorophenoxy)diphenylsilane
701266-72-0P, [3-(tert-Butvldiphenvlsilanvloxv)-2,6-
difluorophenyl] (hydroxy) acetic acid ethyl ester 701266-73-1P,
[3-(tert-Butyldiphenylsilanyloxy)-2,6-difluorophenyl](ethoxy)acetic acid
ethvl ester
             701266-74-2P, (2.6-Difluoro-3-hydroxyphenyl) (ethoxy) acetic
      701266-75-3P, (2,6-Difluoro-3-hydroxyphenyl) (ethoxy) acetic acid
            701266-76-4P, [[4-[[[2-(2,6-Difluoro-3-hydroxyphenyl])-2-
ethyl ester
ethoxyacetyl|amino|methyl|phenyl|(imino)methyl|carbamic acid benzyl ester
701267-11-0P, [2,6-Difluoro-3-(4-fluorophenoxy)phenyl](ethoxy)acetic acid
ethvl ester
              701267-13-2P, [2,6-Difluoro-3-(4-
fluorophenoxy)phenyl](ethoxy)acetic acid
                                          701267-14-3P
                                                        701267-20-1P.
N-(4-Cyanobenzyl)-2-(2,6-difluoro-3-hydroxyphenyl)-2-ethoxyacetamide
701267-21-2P, N-(4-Cyanobenzyl)-2-ethoxy-2-[3-(1-ethylpropoxy)-2,6-
                         701267-28-9P, Trifluoromethanesulfonic acid
difluorophenvl|acetamide
3-[(4-cvanobenzylcarbamovl)(ethoxy)methyl]-2,4-difluorophenyl ester
701267-29-0P, N-(4-Cyanobenzyl)-2-[2,6-difluoro-3-(pyridin-2-yl)phenyl]-2-
ethoxyacetamide
                701267-30-3P, 2-[2,6-Difluoro-3-(pyridin-2-yl)phenyl]-2-
ethoxy-N-[4-(N-hydroxycarbamimidoyl)benzyl]acetamide
                                                      701267-37-0P,
[3-(tert-Butyldiphenylsilanyloxy)-2,6-difluorophenyl] (methoxy) acetic acid
             701267-39-2P, (2,6-Difluoro-3-hydroxyphenyl) (methoxy) acetic
ethyl ester
                  701267-40-5P, (2,6-Difluoro-3-
acid ethyl ester
                                    701267-41-6P.
hydroxyphenyl) (methoxy) acetic acid
N-(4-Cyanobenzyl)-2-(2,6-difluoro-3-hydroxyphenyl)-2-methoxyacetamide
701267-42-7P, Trifluoromethanesulfonic acid
3-[(4-cyanobenzylcarbamoyl)(methoxy)methyl]-2,4-difluorophenyl ester
701267-51-8P, 3-[(4-Cyanobenzylcarbamoyl)(methoxy)methyl]-2,4-
difluorobenzoic acid methyl ester
                                   701267-52-9P,
3-[(4-Cvanobenzylcarbamov1) (methoxy)methyl]-2,4-difluorobenzoic acid
701267-53-0P, 2-[2,6-Difluoro-3-[(morpholin-4-v1)carbonv1]phenv1]-N-[4-(N-
hydroxycarbamimidoyl)benzyl]-2-methoxyacetamide
                                                701267-71-2P,
N-(4-Cyanobenzyl)-2-[2,6-difluoro-3-(4-fluorophenoxy)phenyl]-2-
                 701267-72-3P, 2-[2,6-Difluoro-3-(4-
methoxyacetamide
fluorophenoxy)phenyl]-N-[4-(N-hydroxycarbamimidoyl)benzyl]-2-
methoxvacetamide
                  701267-75-6P, N-(4-Cvanobenzyl)-2-(3,5-difluorobiphenyl-
4-v1)-2-methoxvacetamide
                          701267-77-8P.
N-(4-Cyanobenzyl)-2-(3,5-difluorobiphenyl-4-yl)-2-ethoxyacetamide
701267-82-5P, N-(4-Cyanobenzyl)-2-[2,6-difluoro-4-(furan-2-yl)phenyl]-2-
ethoxyacetamide
                 701267-83-6P, 2-[2,6-Difluoro-4-(furan-2-yl)phenyl]-2-
ethoxy-N-[4-(N-hydroxycarbamimidoy1)benzy1]acetamide
                                                      701267-89-2P,
[[4'-[(4-Cyanobenzylcarbamoy1)(ethoxy)methy1]-3',5'-difluorobipheny1-3-
yl]oxy]acetic acid ethyl ester
                                701267-91-6P,
[[4'-[(4-Carbamimidoylbenzylcarbamoyl)(ethoxy)methyl]-3',5'-
difluorobiphenyl-3-ylloxylacetic acid ethyl ester hydrochloride
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701268-01-1P, N-(4-Cyanobenzyl)-2-(3,5-difluoro-2'-hydroxybiphenyl-4-yl)-2-
    ethoxyacetamide 701268-03-3P, 2-12'-(2-Benzyloxyethoxy)-3,5-
                                                                  701268-08-8P.
    difluorobiphenyl-4-yl|-N-(4-cyanobenzyl)-2-ethoxyacetamide
    N-(4-Cyanobenzyl)-2-[2'-(2-dimethylaminoethoxy)-3,5-difluorobiphenyl-4-yl]-
    2-ethoxyacetamide
                       701268-18-0P
, 2-[2'-(Carbamoylmethoxy)-3,5-difluorobiphenyl-4-yl]-2-ethoxy-N-[4-(N-
    hydroxycarbamimidoyl)benzyl]acetamide 701268-23-7P,
    N-(4-Cyanobenzyl)-2-[2,6-difluoro-4-(4,4,5,5-tetramethyl-
    [1,3,2]dioxaborolan-2-v1)phenv1]-2-ethoxvacetamide 701268-25-9P,
    N-(4-Cvanobenzyl)-2-[2,6-difluoro-4-(pyridin-4-yl)phenyl]-2-
    ethoxyacetamide 701268-48-6P, [Amino[4-[[[2-[4-(6-aminopyridin-3-yl)-2,6-
    difluorophenyl]-2-ethoxyacetyl]amino]methyl]phenyl]methylenelcarbamic acid
    ethyl ester 701268-52-2P, N-(4-Cyanobenzyl)-2-(3,5-difluoro-2'-
    formylbiphenyl-4-yl)-2-ethoxyacetamide 701268-54-4P,
    N-(4-Cyanobenzyl)-2-(3,5-difluoro-2'-hydroxymethylbiphenyl-4-yl)-2-
    ethoxyacetamide 701268-59-9P, 2-[3,5-Difluoro-2'-
     [hydroxy(imino)methyl]biphenyl-4-yl]-2-ethoxy-N-[4-(N-
    hydroxycarbamimidoyl)benzyl]acetamide 701268-62-4P,
    3-Benzyloxy-2-fluoro-4-methoxybenzaldehyde 701268-63-5P,
     (3-Benzyloxy-2-fluoro-4-methoxyphenyl) (methoxy) acetic acid
                                                                  701268-65-7P,
    N-(4-Cyanobenzyl)-2-(2-fluoro-3-hydroxy-4-methoxyphenyl)-2-
    methoxyacetamide 701268-67-9P, N-(4-Cyanobenzyl)-2-(2-fluoro-4-methoxy-3-
    phenoxyphenyl)-2-methoxyacetamide 701268-72-6P, Trifluoromethanesulfonic
    acid 2-1(4-cvanobenzylcarbamovl) (methoxy)methyll-3-fluorophenyl ester
    701268-74-8P, N-(4-Cyanobenzyl)-2-[2-fluoro-6-
     [(trimethylsilanyl)ethynyl]phenyl]-2-methoxyacetamide
                                                            701268-77-1P.
    N-(4-Cyanobenzy1)-2-[2-fluoro-6-[3-[(tetrahydropyran-2-y1)oxy]prop-1-
                                     701268-80-6P,
    vnvllphenvll-2-methoxvacetamide
    N-(4-Cvanobenzvl)-2-(3-fluorobiphenvl-2-vl)-2-methoxyacetamide
    701268-86-2P, [2-[(4-Cyanobenzylcarbamoy1)(methoxy)methy1]-3-
    fluorophenoxy]acetic acid methyl ester
                                             701268-92-0P.
     (4-Benzyloxy-2,6-difluorophenyl) (ethoxy) acetic acid
                                                          701268-93-1P,
     2-(4-Benzyloxy-2,6-difluorophenyl)-N-(4-cyanobenzyl)-2-ethoxyacetamide
    701268-95-3P, N-(4-Cvanobenzyl)-2-(2,6-difluoro-4-hydroxyphenyl)-2-
                     701268-97-5P, N-(4-Cyanobenzyl)-2-(2,6-difluoro-4-
    ethoxvacetamide
    isopropoxyphenyl)-2-ethoxyacetamide 701269-10-5P,
    N-(4-Cyanobenzyl)-2-(2,6-difluoro-4-phenoxyphenyl)-2-ethoxyacetamide
    RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
       (intermediate; preparation of N-(carbamimidovlbenzyl) benzeneacetamides and
       pyridineacetamides as coagulation factor inhibitors)
    701269-21-8P, (2,4-Difluorophenyl)carbamic acid tert-butvl ester
    701269-22-9P, (2,4-Difluoro-3-formylphenyl)carbamic acid tert-butyl ester
    701269-23-0P, [3-[(tert-Butoxycarbonyl)amino]-2,6-
    difluorophenyl] (methoxy) acetic acid
                                          701269-24-1P,
    [3-[(4-Cvanobenzylcarbamovl)(methoxy)methyl]-2,4-difluorophenyl]carbamic
                           701269-25-2P,
    acid tert-butvl ester
    2-(3-Amino-2,6-difluorophenyl)-N-(4-cyanobenzyl)-2-methoxyacetamide
    701269-26-3P, N-(4-Cyanobenzyl)-2-(2,6-difluoro-3-phenylaminophenyl)-2-
                        701269-27-4P, 2-(2,6-Difluoro-3-phenylaminophenyl)-N-[4-
    methoxyacetamide
    (N-hydroxycarbamimidoyl)benzyl]-2-methoxyacetamide
                                                         701269-30-9P,
    N-(4-Cyanobenzyl)-2-(2,6-difluoro-3-isopropylaminophenyl)-2-
                        701269-35-4P, 2-(2,4-Difluorophenvl)-[1,3]dioxolane
    methoxvacetamide
    701269-36-5P, (2,6-Difluoro-3-formylphenyl)(ethoxy)acetic acid 701269-37-6P, N-(4-Cyanobenzyl)-2-(2,6-difluoro-3-formylphenyl)-2-
    et.hoxvacet.amide
                     701269-38-7P, N-(4-Cyanobenzyl)-2-(2,6-difluoro-3-
    hydroxymethylphenyl)-2-ethoxyacetamide
                                             701269-40-1P,
    N-(4-Cyanobenzy1)-2-[2,6-difluoro-3-[hydroxy(imino)methyl]pheny1]-2-
    ethoxyacetamide
                       701269-42-3P, 2-(3-Aminomethyl-2,6-difluorophenyl)-N-(4-
    cyanobenzyl)-2-ethoxyacetamide acetate 701269-43-4P,
    2-[3-[(Acetylamino)methyl]-2,6-difluorophenyl]-N-(4-cyanobenzyl)-2-
    ethoxyacetamide 701269-45-6P, 2-[2,6-Difluoro-3-
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[hydroxy(imino)methyl]phenyl]-2-ethoxy-N-[4-(N-
hydroxycarbamimidov1)benzyllacetamide 701269-48-9P,
N-(4-Cyanobenzy1)-2-[2,6-difluoro-3-[(phenylamino)methyl]phenyl]-2-
ethoxvacetamide
                 701269-55-8P, 4-Aminomethyl-3,5-difluorobenzonitrile
              701269-56-9P, N-(4-Cyano-2,6-difluorobenzy1)-2-(2,6-
hvdrochloride
difluoro-4-methoxyphenyl)-2-ethoxyacetamide
                                            701269-64-9P
                                                           701269-65-0P.
4-Aminomethyl-3-nitrobenzonitrile 701269-66-1P,
N-(4-Cyano-2-nitrobenzyl)-2-ethoxy-2-(2-fluoro-4-methoxyphenyl)acetamide
701269-67-2P, N-(2-Amino-4-cvanobenzvl)-2-ethoxy-2-(2-fluoro-4-
methoxyphenyl)acetamide 701269-68-3P.
N-[2-[(Carbamoylmethyl)amino]-4-cyanobenzyl]-2-ethoxy-2-(2-fluoro-4-
methoxyphenyl)acetamide 701269-79-6P,
N-[4-Cyano-2-[(phenylmethylsulfonyl)amino]benzyl]-2-ethoxy-2-(2-fluoro-4-
methoxyphenyl)acetamide 701269-84-3P,
N-(4-Cyano-2-phenylaminobenzyl)-2-ethoxy-2-(2-fluoro-4-
methoxyphenyl)acetamide 701269-86-5P,
[2,6-Difluoro-4-(4,4,5,5-tetramethyl-[1,3,2]dioxaborolan-2-
yl)phenyl](ethoxy)acetic acid ethyl ester 701269-87-6P,
[4-(6-Aminopyridin-3-yl)-2,6-difluorophenyl](ethoxy)acetic acid
701269-88-7P, 2-[4-(6-Aminopyridin-3-y1)-2,6-difluoropheny1]-N-[2-
(carbamovlmethoxy)-4-cyanobenzyl]-2-ethoxyacetamide 701269-90-1P,
[2,6-Difluoro-4-(pyridin-2-vlmethoxy)phenyl](ethoxy)acetic acid
701269-91-2P, N-[2-(Carbamovlmethoxy)-4-cyanobenzyl]-2-[2,6-difluoro-4-
[(pyridin-2-y1)methoxy]pheny1]-2-ethoxyacetamide
                                                  701269-93-4P.
2-[4-(6-Aminopyridin-3-yl)-2,6-difluorophenyl]-N-(4-cyano-2,6-
                                  701270-05-5P,
difluorobenzyl)-2-ethoxyacetamide
Ethoxy(2-fluoro-4-methoxyphenyl)acetic acid ethyl ester
                                                        701270-07-7P.
(R)-Ethoxy(2-fluoro-4-methoxyphenyl)ethanoic acid 701270-12-4P,
(2,6-Difluoro-4-hydroxyphenyl) (methoxy) acetic acid ethyl ester
701270-13-5P, [2,6-Difluoro-4-(4,4,5,5-tetramethyl-[1,3,2]dioxaborolan-2-
yl)phenyl](methoxy)acetic acid ethyl ester 701270-14-6P,
[2,6-Difluoro-4-(pyridin-4-yl)phenyl] (methoxy) acetic acid ethyl ester
701270-15-7P, [2,6-Difluoro-4-(1-oxopyridin-4-yl)phenyl] (methoxy) acetic
                  701270-16-8P, [2,6-Difluoro-4-(1-oxopyridin-4-
acid ethvl ester
vl)phenvll(methoxv)acetic acid
                                701270-19-1P,
N-(4-Cyanobenzyl)-2-[4-(3,6-dihydro-2H-pyran-4-yl)-2,6-difluorophenyl]-2-
ethoxyacetamide
                701272-56-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
  (intermediate; preparation of N-(carbamimidovlbenzyl) benzeneacetamides and
  pyridineacetamides as coagulation factor inhibitors)
9002-04-4, Thrombin 9002-05-5, Factor Xa 9035-58-9, Tissue factor
(blood-coagulation) 14708-95-3D, Factor III, complex with factor VIIa
37316-87-3, Factor IXa
                       65312-43-8, Factor VIIa 65312-43-8D, Factor
VIIa, complex with factor III
RL: BSU (Biological study, unclassified); BIOL (Biological study)
   (preparation of N-(carbamimidovlbenzvl)benzeneacetamides and
  pyridineacetamides as coagulation factor inhibitors)
60-12-8, Phenethyl alcohol
                           62-53-3, Aniline, reactions
                                                         67-36-7,
                      75-30-9, 2-Iodopropane 78-81-9, Isobutylamine
4-Phenoxybenzaldehyde
                   89-98-5, 2-Chlorobenzaldehyde
78-83-1, reactions
                                                    96-30-0,
2-Chloro-N-methylacetamide
                           96-41-3, Cyclopentanol
                                                    97-99-4,
                           98-80-6, Phenylboronic acid
Tetrahydrofurfurvl alcohol
                                                          98-86-2,
Acetophenone, reactions 99-61-6, 3-Nitrobenzaldehyde
4-Dimethylaminobenzaldehyde 100-52-7, Benzaldehyde, reactions
100-55-0, 3-(Hydroxymethyl)pyridine 100-97-0, reactions
                                                           103-74-2.
2-(2-Hydroxyethyl)pyridine 105-36-2, Ethyl bromoacetate
                                                           106-52-5.
4-Hydroxy-N-methylpiperidine 108-01-0, 2-Dimethylaminoethanol
108-93-0, Cyclohexanol, reactions 108-95-2, Phenol, reactions
109-85-3, 2-Methoxyethylamine 109-86-4, 2-Methoxyethanol
Diethylamine, reactions 110-80-5, 2-Ethoxyethanol 110-91-8,
Morpholine, reactions 111-90-0, Diethylene glycol monoethyl ether
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112-35-6, Triethylene glycol monomethyl ether 120-57-0, Piperonal 122-85-0, 4-Acetamidobenzaldehyde 122-99-6, 2-Phenoxyethanol 285-67-6,
Cyclopentene oxide
                   331-64-6, 2-Fluoro-4-methoxybenzaldehyde 348-27-6,
2-Fluoro-4-hydroxybenzaldehyde 367-27-1, 2,4-Difluorophenol 437-81-0,
2,6-Difluorobenzaldehyde 446-52-6, 2-Fluorobenzaldehyde 456-22-4,
4-Fluorobenzoic acid 461-96-1, 1-Bromo-3,5-difluorobenzene 501-53-1,
                     513-38-2, 1-Iodo-2-methylpropane 541-41-3, Ethyl
Benzyl chloroformate
chloroformate 586-95-8, 4-(Hydroxymethyl)pyridine 586-98-1,
2-Hydroxymethylpyridine 622-08-2, 2-Benzyloxyethanol 622-40-2,
N-(2-Hydroxyethyl)morpholine 626-55-1, 3-Bromopyridine 659-28-9,
4-(Trifluoromethoxy)benzaldehyde 873-74-5, 4-Aminobenzonitrile
924-44-7 1066-54-2, (Ethynyl)trimethylsilane 1072-97-5,
2-Amino-5-bromopyridine 1121-60-4, 2-Pyridinecarboxaldehyde
                                                             1204-86-0.
4-(Morpholino)benzaldehyde 1423-26-3, [3-(Trifluoromethyl)phenyl]boronic
acid 1484-84-0, 2-Piperidineethanol 1550-35-2,
2,4-Difluorobenzaldehyde 1583-58-0, 2,4-Difluorobenzoic acid
1700-37-4, 3-Benzyloxybenzaldehyde 1765-93-1, 4-Fluorobenzeneboronic
     1809-10-5, 3-Bromopentane 1939-99-7, Benzylsulfonyl chloride
2081-44-9, Tetrahydro-2H-pyran-4-ol 2240-88-2,
3,3,3-Trifluoro-1-propanol 2516-33-8, Hydroxymethylcyclopropane
2516-47-4, Aminomethylcyclopropane 2566-44-1, 2-Cyclopropylethanol
2629-72-3, 3-(4-Pyridyl)propanol 2646-91-5, 2,3-Difluorobenzaldehyde
2713-34-0, 3,5-Difluorophenol 2746-14-7, (1-Methylcyclopropyl)methanol
2916-68-9, 2-(Trimethylsilyl)ethanol 2955-88-6,
1-(2-Hydroxyethyl)pyrrolidine 3040-44-6, 1-(2-Hydroxyethyl)piperidine
3143-02-0, 3-Methyl-3-oxetanemethanol 3173-56-6, Benzyl isocyanate
3179-63-3
          3218-36-8, 4-Biphenylaldehyde 3445-11-2,
N-(2-Hydroxyethyl)-2-pyrrolidone 3453-33-6, 6-Methoxy-2-naphthaldehyde
3601-66-9 3966-32-3, (R)-\alpha-Methoxybenzeneethanoic acid
4397-53-9, 4-Benzyloxybenzaldehyde 4415-82-1, Cyclobutylmethanol
4548-45-2, 2-Chloro-5-nitropyridine 4584-46-7,
1-Chloro-2-dimethylaminoethane hydrochloride
                                             4595-59-9,
                  4856-97-7, 1H-Benzimidazole-2-methanol
                                                            4870-65-9.
5-Bromopyrimidine
α-Bromobenzeneacetic acid 5402-55-1, 2-(2-Thienv1)ethanol
5720-05-8, 4-Methylbenzeneboronic acid 5720-06-9, 2-Methoxyphenylboronic
      5720-07-0, 4-Methoxyphenylboronic acid 6077-72-1,
(2-Methylcyclopropyl)methanol 6089-04-9,
Tetrahydro-2-(2-propynyloxy)-2H-pyran
                                     6244-54-8,
2-(Biphenyl-4-yl)-2-hydroxypropionic acid 6293-56-7,
3-(2-Hydroxyethyl)pyridine 6346-05-0, 3-Benzyloxy-4-methoxybenzaldehyde
6630-33-7, 2-Bromobenzaldehyde
                               7583-53-1, 1-Methvl-3-piperidinemethanol
7589-27-7, 4-Fluorophenethyl alcohol 7677-24-9, Trimethylsilyl cyanide
10040-98-9, 1-(4-Formylphenyl)-1H-imidazole 10365-98-7,
3-Methoxyphenylboronic acid 10406-25-4, 4-Aminomethylbenzonitrile
13331-23-2, 2-Furanboronic acid 13472-85-0, 5-Bromo-2-methoxypyridine
15854-87-2, 4-Iodopyridine 15996-76-6, 4-Aminomethylbenzonitrile
hydrochloride 17392-83-5, Methyl (R)-(+)-lactate
                                                   17933-03-8,
m-Tolylboronic acid 19059-68-8, 3-Dimethylamino-2,2-dimethyl-1-propanol
19524-06-2, 4-Bromopyridine hydrochloride
                                          20845-34-5.
1-Methyl-2-piperidinemethanol 25494-07-9
                                          26164-26-1,
(S)-α-Methoxybenzeneethanoic acid 26934-35-0,
4-[3-(Dimethylamino)propoxy]benzaldehyde 28611-39-4,
(4-Dimethylaminophenyl)boronic acid 32884-23-4,
                                  39096-01-0,
2-Benzyloxy-4-methoxybenzaldehyde
N,N-Diethyl-2-hydroxyacetamide 39515-51-0, 3-Phenoxybenzaldehyde
51791-12-9, 3-(Chloromethyl)-1,2,4-oxadiazole 51980-54-2,
4-(Pyrrolidino)benzaldehyde
                            54439-75-7, 2-Chloro-4-methoxybenzaldehyde
57848-46-1, 4-Bromo-2-fluorobenzaldehyde 58028-76-5,
2-(Morpholino)benzaldehyde 58479-61-1, tert-Butyldiphenylchlorosilane
59664-42-5, 2,4-Bis(trifluoromethyl)benzaldehyde 61370-75-0,
2,2-Dimethylchromane-6-carboxaldehyde 63628-25-1,
2-Methoxy-2-(1-naphthyl)propionic acid 67387-76-2,
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3-(Cyclopentyloxy)-4-methoxybenzaldehyde
                                                71924-62-4.
     6-Fluoroveratraldehyde
                             73183-34-3 79418-73-8,
     2-Fluoro-3-hydroxy-4-methoxybenzaldehyde 81655-41-6
                                                             84102-89-6.
     4-Formvl-3-hvdroxybenzonitrile 87199-18-6, 3-Hvdroxyphenylboronic acid
     89466-08-0, 2-Hydroxyphenylboronic acid 89763-93-9,
     2-Fluoro-4-(trifluoromethyl)benzaldehyde 93249-44-6,
     2-Fluoro-5-methylbenzaldehyde
                                   93343-10-3, 3,5-Difluoroanisole
     93777-26-5, 5-Bromo-2-fluorobenzaldehyde
                                                98546-51-1,
     4-(Methylthio)phenylboronic acid 103438-88-6,
     2-Fluoro-3-methoxybenzaldehyde 105942-09-4,
     4-(Bromomethyl)-3-fluorobenzonitrile 105942-10-7,
     3-Fluoro-4-formylbenzonitrile 109384-19-2,
     1-tert-Butoxycarbonyl-4-hydroxypiperidine
     2-Fluoro-6-methoxybenzaldehyde 146137-78-2,
     5-(Trifluoromethyl)-2-fluorobenzaldehyde 162698-22-8,
     [(Amino)(4-aminomethylphenyl)methylene]carbamic acid benzyl ester
     hydrochloride 172348-75-3, [(4-Aminomethylphenyl)(imino)methyl]carbamic
     acid benzyl ester dihydrochloride 176175-97-6,
     1-Benzyloxy-3,5-difluorobenzene 182159-14-4,
     4-Aminomethyl-3-methoxybenzonitrile
                                         188975-30-6,
     Trifluoromethanesulfonic acid 3,6-dihydro-2H-pyran-4-vl ester
     200195-15-9, 3-0xo-3,4-dihydro-2H-benzo[1,4]oxazine-6-carboxaldehyde
     202521-97-9, 4-Aminomethyl-3-chlorobenzonitrile
                                                      202522-15-4,
     4-Aminomethyl-2-chlorobenzonitrile 223512-70-7.
     4-Bromomethyl-3-nitrobenzonitrile 256417-10-4,
     2,6-Difluoro-4-methoxybenzaldehyde 277324-21-7, 3,5-Diethoxy-2-fluorobenzaldehyde 368426-73-7,
     4-Aminomethvl-2-fluorobenzonitrile 376600-66-7,
     5-Ethoxy-2-fluoro-4-(2-hydroxyethoxy)benzaldehyde
                                                        467442-15-5,
     3.5-Difluoro-4-formylbenzonitrile 701263-50-5.
     5-Ethoxy-2-fluoro-3-(1-methylpiperidin-4-yloxy)benzaldehyde
                                                                  701263-78-7,
     (3-Benzyloxyphenyl) (methoxy) acetic acid 701263-88-9,
     N-(4-Cyanobenzyl)-2-(3-hydroxyphenyl)-2-methoxyacetamide
                                                                701263-96-9,
     3,4-Diethoxy-2-fluorobenzaldehyde
                                       701264-46-2,
     2-(4-Bromo-2-fluorophenyl)-N-(4-cyanobenzyl)-2-methoxyacetamide
     701265-02-3, O-Benzyl-3-fluorobenzene 701265-37-4,
     4-(5-Ethoxy-2-fluoro-3-formylphenoxy)piperidine-1-carboxylic acid
     tert-butyl ester
                       701267-79-0, 2-(4-Bromo-2,6-difluorophenyl)-N-(4-
     cyanobenzyl)-2-ethoxyacetamide
                                     701269-03-6,
     N-(4-Cyanobenzyl)-2-[2,6-difluoro-4-[(pyridin-2-yl)methoxy]phenyl]-2-
                       701269-52-5 701270-17-9, 4-Aminomethylbenzamidine
     ethoxvacetamide
     hydrochloride
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (preparation of N-(carbamimidoylbenzyl)benzeneacetamides and
        pyridineacetamides as coaqulation factor inhibitors)
RE.CNT 13
             THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD
(1) Anon: WO 0035858 A1 CAPLUS
(2) Anon: WO 0168605 A1 CAPLUS
(3) Anon; WO 0190051 A1 CAPLUS
(4) Anon; WO 0192214 A1 CAPLUS
(5) Anon; WO 02062829 A1 CAPLUS
(6) Anon; WO 0210127 A1 CAPLUS
(7) Anon; WO 0216315 A1 CAPLUS
(8) Anon; WO 0228823 A1
(9) Anon; WO 0234711 A1 CAPLUS
(10) Anon; WO 0237937 A2 CAPLUS
(11) Anon; WO 03020710 A1 CAPLUS
(12) Anon; EP 0921116 A1 CAPLUS
(13) Anon; EP 1078917 A1 CAPLUS
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RE

- AN 2003:487141 CAPLUS
- DN 139:53457
- ED Entered STN: 26 Jun 2003
 - Procedure for the anhydrous production of formic acid and (meth)acrylate esters by the transesterification of formate esters and (meth)acrylic acids
- Zehner, Peter; Pastre, Joerg; Stueer, Wolfram; Machhammer, Otto; IN Schroeder, Juergen
- PA BASF A.-G., Germany
- SO Ger. Offen., 10 pp. CODEN: GWXXBX
- DT Pat.ent.
- LA German
- TC: ICM C07C027-00
- ICS C07C067-02; C07C051-09; C07C053-02; C07C069-54

KIND DATE

CC 35-2 (Chemistry of Synthetic High Polymers)

Section cross-reference(s): 23, 48 FAN CHT 1

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	107	TENT	MO

IIIIIIII 110.		TITLE	DITTE	THE DECITE OF THE	DILLE
PRAI DE 2002-102		A1	20030626 20020704	DE 2002-10230221	20020704
PATENT NO.	CLASS	PATENT	FAMILY CLASS	IFICATION CODES	
DE 10230221	ICM ICS IPCI	C07C067 C07C002 [ICS,7, C07C005	7-02; C07C051 7-00 [ICM,7] C*]; C07C005 3-00 [ICS,7,	; C07C0067-02 [ICS,7]; 1-09 [ICS,7]; C07C0053 C*]; C07C0069-54 [ICS,	C07C0067-00 3-02 [ICS,7];
	IPCR				7C0067-00
	ECLA	C07C051	/09+53/02; C	07C067/10+69/54	
	PI DE 10230221 PRAI DE 2002-102 CLASS PATENT NO.	PI DE 10230221 PRAI DE 2002-10230221 CLASS PATENT NO. CLASS DE 10230221 ICM ICS IPCI	PI DE 10230221 A1 PRAI DE 2002-10230221 CLASS PATENT NO. CLASS PATENT DE 10230221 ICM C07C027 ICS C07C006 IPCI C07C006 07C006 IPCR C07C006 IPCR C07C006 IPCR C07C006 IPCR C07C006 IPCR C07C006 IPCR C07C006 IPCR IT,C*1,1	PI DE 10230221 A1 20030626 PRAI DE 2002-10230221 20020704 CLASS PATENT NO. CLASS PATENT FAMILY CLASS DE 10230221 ICM C07C027-00 ICS C07C067-02; C07C051 IPCI C07C0027-00 [ICM, 7] ICS, 7,C*]; C07C005 C07C0053-00 [ICS,7, C07C0050-00] I,C*]; IPCR C07C0051-09 I,C*]; IIPCR C07C0051-09 I,	PI DE 10230221 A1 20030626 DE 2002-10230221 PRAI DE 2002-10230221 20020704 CLASS PATENT FAMILY CLASSIFICATION CODES DE 10230221 ICM C07C027-00 ICS C07C067-02; C07C051-09; C07C053-02; C07C051-02 IPCI C07C0027-00 [ICM,7]; C07C0067-02 [ICS,7]; ICS,7,C*]; C07C0051-09 [ICS,7]; C07C0055-04 [ICS, C07C0051-09] ICS,7]; C07C0055-09 [ICS,7]; C07C0055-09 [I,A]; C07C0055-09 [I,C*]; C07C0055-09 [I,A];

APPLICATION NO

ECLA

- OS MARPAT 139:53457 AR Formic acid and (meth)acrylate esters (e.g., Me acylate) are
- prepared by the transesterification of a formate ester (e.g., Me formate) with (meth)acrylic acids (e.g., acrylic acid), and the (meth) acrylate ester is then transesterified with a higher alc.
- methyl acrylate manuf transesterification formate ester acrylic acid; alkyl methacrylate manuf transesterification formate ester methacrylic acid
- Transesterification catalysts

(acid cation exchangers; procedure for the anhydrous production of formic acid and (meth)acrylate esters by the transesterification of formate esters and (meth)acrylic acids using)

- Carboxvlic acids, reactions
 - RL: RCT (Reactant); RACT (Reactant or reagent)

(esters, alkyl formates; procedure for the anhydrous production of formic acid and (meth)acrylate esters by the

transesterification of formate esters and (meth)acrylic acids)

- Transesterification
 - (procedure for the anhydrous production of formic acid and (meth)acrylate esters by the transesterification of formate esters and (meth)acrylic acids)
- 11138-38-8, Lewatit S100
 - RL: CAT (Catalyst use); USES (Uses)

(catalyst; procedure for the anhydrous production of formic acid and (meth)acrylate esters by the transesterification of formate esters and (meth)acrylic acids)

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71-36-3, 1-Butanol, reactions 71-41-0, 1-Pentanol, reactions 77-99-6, Trimethylolpropane 100-37-8, 2-(Diethylamino)ethanol 102-81-8,
     2-(Dibutylamino)ethanol 104-76-7, 2-Ethylhexanol 108-01-0, 2-(
     Dimethylamino)ethanol 110-63-4, 1,4-Butanediol,
     reactions 111-87-5, 1-Octanol, reactions 115-77-5, Pentaerythritol,
     reactions 143-08-8, 1-Nonanol 629-11-8, 1,6-Hexanediol 24800-44-0,
     Tripropylene glycol 25265-71-8, Dipropylene glycol
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (in a procedure for the anhydrous production of formic acid and
        (meth)acrylate esters by the transesterification of formate
        esters and (meth)acrylic acids)
     64-18-6P. Formic acid, preparation
     RL: BYP (Byproduct); PREP (Preparation)
        (procedure for the anhydrous production of formic acid and
        (meth)acrylate esters by the transesterification of formate
        esters and (meth)acrylic acids)
     80-62-6P, Methyl methacrylate 96-33-3P, Methyl acrylate
     RL: IMF (Industrial manufacture); PREP (Preparation)
        (procedure for the anhydrous production of formic acid and
        (meth)acrylate esters by the transesterification of formate
        esters and (meth)acrylic acids)
     107-31-3P, Methyl formate
     RL: PNU (Preparation, unclassified); RCT (Reactant); PREP (Preparation);
     RACT (Reactant or reagent)
        (procedure for the anhydrous production of formic acid and
        (meth)acrylate esters by the transesterification of formate
        esters and (meth)acrylic acids)
     79-10-7, Acrylic acid, reactions 79-41-4, Methacrylic acid, reactions
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (procedure for the anhydrous production of formic acid and
        (meth)acrylate esters by the transesterification of formate
        esters and (meth)acrylic acids)
    ANSWER 21 OF 55 CAPLUS COPYRIGHT 2009 ACS on STN
L9
AN 2002:944826 CAPLUS
DN
    138:25860
ED
    Entered STN: 13 Dec 2002
TI Lead-free cationic electrodeposition coating compositions containing
    crosslinked resin particles
TN
    Kojima, Yoshio; Uchidoi, Satoru; Yamada, Mitsuo
PA Nippon Paint Co., Ltd., Japan
SO Jpn. Kokai Tokkvo Koho, 14 pp.
    CODEN: JKXXAF
DT Patent
LA
    Japanese
TC
    ICM C09D163-00
     ICS C09D005-44; C09D133-12; C09D133-14; C09D175-04; C25D013-06;
          C25D013-10
     42-9 (Coatings, Inks, and Related Products)
FAN.CNT 1
     PATENT NO.
                         KIND
                                DATE
                                           APPLICATION NO.
    JP 2002356646
                                20021213
                                           JP 2001-164399
                                                                  20010531
PRAI JP 2001-164399
                                20010531
CLASS
 PATENT NO. CLASS PATENT FAMILY CLASSIFICATION CODES
 JP 2002356646
                 TCM
                        C09D163-00
                 TCS
                        C09D005-44; C09D133-12; C09D133-14; C09D175-04;
                        C25D013-06; C25D013-10
                 IPCI C09D0163-00 [ICM, 7]; C09D0005-44 [ICS, 7]; C09D0133-12
                        [ICS,7]; C09D0133-10 [ICS,7,C*]; C09D0133-14 [ICS,7];
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C09D0175-04 [ICS,7]; C25D0013-06 [ICS,7]; C25D0013-04 [ICS,7,7c*]; C25D0013-10 [ICS,7] [ICS,7]; C25D0013-10 [ICS,7] [I

- AB The compns. have a min. film-forming temperature of 20--30, are based on (A) cationic polymers comprising a 10--90--90--10 mixture of amine-modified epoxy resins (A1) and sulfonium-modified epoxy resins (A2) and crosslinkers (blocked polyisocyanates), and contain 3--20--10 (based on resins in A) crosslinked resin particles prepared from α , β -unsatd. monomers in the presence of ammonium group-containing acrylic polymers as emulsifiers, where the amine groups of A1 have been neutralized with acids (HCOOH) to 5--30 mequiv per 100 g of resin and crosslinker, and the sulfonium group content is at 5--30 mequiv is 10--30 mequiv.
- ST cationic deposition coating modified epoxy resin blocked polyisocyanate crosslinker
- IT Electrodeposition

(cationic; lead-free cationic deposition coating compns. for use on metal sheets with freedom from pinholes and crater)

IT Polymerization

(emulsion; manufacture of lead-free cationic electrodeposition coating compns. containing crosslinked resin particles)

IT Galvanized steel

RL: MSC (Miscellaneous)

(sheet metals; manufacture of lead-free cationic electrodeposition coating compns. containing crosslinked resin particles)

IT 91-08-7DP, 2,6-TDI, blocked derivative 101-68-8DP, MDI, blocked derivative 584-84-9DP, 2,4-TDI, blocked derivative 4098-71-9DP, IPDI, blocked derivative RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)

(crosslinker; lead-free cationic deposition coating compns. for use on metal sheets with freedom from pinholes and crater)

IT 108-01-0DP, N,N-Dimethylaminoethanol, reaction products with glycidyl methacrylate copolymer

RL: IMF (Industrial manufacture); MOA (Modifier or additive use); PREP (Preparation); USES (Uses)

(emulsifiers; manufacture of lead-free cationic electrodeposition coating compns. containing crosslinked resin particles)

IIT 443762-01-4DP, Butyl methacrylate-2-ethylhexyl methacrylate-glycidyl methacrylate-2-nydroxyethyl methacrylate copolymer, reaction products with dimethylaminoethanol

RL: IMF (Industrial manufacture); POF (Polymer in formulation); PRP (Properties); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)

(emulsifiers; manufacture of lead-free cationic electrodeposition coating compns. containing crosslinked resin particles)

II 108-01-0DP, Dimethylethanolamine, cationic derivs. with epoxy resins 11-42-2DP, Diethanolamine, cationic derivs. with epoxy resins 6713-03-7DP, SHP 100 (sulfide), reaction products with epoxy resins 25068-38-6DP, Bisphenol A-epichlorohydrin copolymer, cationic derivs. RL: IMF (Industrial manufacture); POF (Polymer in formulation); PRP (Properties); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)

(lead-free cationic deposition coating compns. for use on metal sheets with freedom from pinholes and crater)

(lead-free cationic deposition coating compns. for use on metal sheets with freedom from pinholes and crater) 50-21-5, Lactic acid, uses 64-18-6, Formic acid, uses 64-19-7, Acetic acid, uses 4767-03-7, Dimethylolpropionic acid 5329-14-6, Sulfamic acid 56743-27-2, Dimethylolbutanoic acid RL: MOA (Modifier or additive use); USES (Uses) (neutralizing agent; lead-free cationic deposition coating compns. for use on metal sheets with freedom from pinholes and crater) 478036-79-2P, Butvl methacrvlate-glycidyl methacrvlate-methyl methacrylate-neopentyl glycol-styrene copolymer RL: IMF (Industrial manufacture); MOA (Modifier or additive use); PREP

(Preparation); USES (Uses)

(particles; manufacture of lead-free cationic electrodeposition coating compns. containing crosslinked resin particles)

- ANSWER 22 OF 55 CAPLUS COPYRIGHT 2009 ACS on STN 1.9
- ΔN 2002:146404 CAPLUS
- DN 137:32937
- ED Entered STN: 26 Feb 2002
- A solvent-free and formalin-free Eschweiler-Clarke methylation of amines
- Rosenau, Thomas; Potthast, Antje; Rohrling, Jurgen; Hofinger, Andreas; AU Sixta, Herbert; Kosma, Paul
- Institute of Chemistry, Christian-Doppler-Laboratory, University of CS Agricultural Sciences, Vienna, Vienna, A - 1190, Austria
- Synthetic Communications (2002), 32(3), 457-465 SO CODEN: SYNCAV; ISSN: 0039-7911
- PB Marcel Dekker, Inc.
- DT Journal
- LA English
- CC 21-2 (General Organic Chemistry)
- OS CASREACT 137:32937
- AB Primary and secondary amines are N-methylated by a mixture of paraformaldehyde and oxalic acid dihydrate in good to excellent yields. The reaction proceeds without involvement of organic solvents and toxic formalin. Reaction temps. of 100° are required for the decomposition of oxalic acid to the intermediate formic acid, which acts as the actual reductant. The reaction conditions have been optimized, and the mechanism has been elucidated by means of deuteration expts.
- ST methylation amine paraformaldehyde oxalic acid dihydrate
- ΤТ Methylation
 - (Eschweiler-Clarke; solvent-free and formalin-free Eschweiler-Clarke methylation of amines)
- Amines, reactions
- RL: RCT (Reactant); RACT (Reactant or reagent) (solvent-free and formalin-free Eschweiler-Clarke methylation of
 - amines) 62-53-3, Aniline, reactions 107-15-3, Ethylenediamine, reactions 110-91-8, Morpholine, reactions 141-43-5, 2-Aminoethanol, reactions 2065-72-7, Oxalic acid-d2 506-59-2, Dimethylamine hydrochloride

dihydrate-d2 6153-56-6, Oxalic acid dihydrate 30525-89-4. 43094-80-0, Paraformaldehyde-d2 Paraformaldehyde

- RL: RCT (Reactant); RACT (Reactant or reagent)
 - (solvent-free and formalin-free Eschweiler-Clarke methylation of amines)
- 108-01-0P, 2-(Dimethylamino)ethanol 109-02-4P, 4-Methylmorpholine 110-18-9P, N,N,N',N'-Tetramethylethylenediamine 121-69-7P, N,N-Dimethylaniline, preparation 593-81-7P, Trimethylamine hydrochloride 134619-42-4P 134619-43-5P

RL: SPN (Synthetic preparation); PREP (Preparation)

- (solvent-free and formalin-free Eschweiler-Clarke methylation of amines)
- RE.CNT 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD

```
(1) Clarke, H; J Am Chem Soc 1933, V55, P4571 CAPLUS
(2) Eschweiler, W; Chem Ber 1905, V38, P880 CAPLUS
(3) Holleman, A: Lehrbuch der anorganischen Chemie: 91-100 Ed 1985, P439
(4) Lapidus, G; Phys Chem 1964, V68, P1863 CAPLUS
(5) Lapidus, G; Phys Chem 1966, V70, P1575 CAPLUS
(6) Lapidus, G; Phys Chem 1966, V70, P3135 CAPLUS
(7) Lapidus, G; Phys Chem 1966, V70, P407 CAPLUS
(8) Leuckardt, R; Ber Dtsch Chem Ges 1885, V18, P2341
(9) Lukasiewicz, A; Tetrahedron 1963, V19, P1789
(10) Rosenau, T; J Org Chem 1999, V64, P2166 CAPLUS
L9
     ANSWER 23 OF 55 CAPLUS COPYRIGHT 2009 ACS on STN
AN
     2001:319483 CAPLUS
DN
     134:315040
ED Entered STN: 04 May 2001
TI Low viscosity, C1-free stabilized hardening accelerators of concrete and
     mortar
     Burge, Theodor A.; Sommer, Marcel; Wombacher, Franz
IN
PA
     Sika A.-G., Vorm. Kaspar Winkler & Co., Switz.
SO
     Eur. Pat. Appl., 12 pp.
     CODEN: EPXXDW
DT
     Patent
LA
     German
IC
     ICM C04B040-00
     ICS C04B022-08; C04B022-14
     58-2 (Cement, Concrete, and Related Building Materials)
FAN. CNT 1
     PATENT NO.
                          KIND DATE
                                               APPLICATION NO.
                                                                       DATE
                                               _____
                          ----
PΤ
     EP 1095922
                          A1 20010502 EP 1999-121549
                                                                      19991029
                          B1
                                 20021211
     EP 1095922
         R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
TE, SI, LT, LV, FI, RO
AT 229487 T 20021215 AT 1999-121549
ES 2186289 T3 20030501 ES 1999-121549
CA 2324393 A1 20010429 CA 2000-2324393
US 6514327 B1 20030204 US 2000-637351
JF 2001180994 A 20010703 JF 2000-330997
JJ 3995877 B2 20071024
AU 200138785 A 20021024 AU 2001-38785
AU 783765 B2 20051201
NZ 511309 A 20030328 NZ 2001-511309
IN 2001MA00353 A 20081128 IN 2001-MA353
PRAI EP 1999-121549 A 19991029
              IE, SI, LT, LV, FI, RO
                                                                        19991029
                                                                        19991029
                                                                        20001024
                                                                        20001027
                                                                        20001030
                                                                        20010423
                                                                        20010424
                                                                        20010501
CLASS
 PATENT NO.
              CLASS PATENT FAMILY CLASSIFICATION CODES
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 EP 1095922
                 ICM C04B040-00
                  ICS
                         C04B022-08; C04B022-14
                        C04B0040-00 [ICM,6]; C04B0022-08 [ICS,6]; C04B0022-14
                  IPCI
                          [ICS,6]; C04B0022-00 [ICS,6,C*]
                   IPCR
                          C04B0022-00 [I,C*]; C04B0022-06 [I,A]; C04B0022-08
                          [I,A]; C04B0022-14 [I,A]; C04B0024-00 [I,C*];
                          C04B0024-02 [I,A]; C04B0024-06 [I,A]; C04B0024-10
                          [I,A]; C04B0024-12 [I,A]; C04B0024-26 [I,A];
                          C04B0024-28 [I,A]; C04B0024-32 [I,A]; C04B0028-00
                          [I,C*]; C04B0028-02 [I,A]; C04B0040-00 [I,C*];
                          C04B0040-00 [I,A]; C04B0103-12 [N,A]; C04B0103-14 [N,A]
                  ECLA C04B022/08; C04B022/14G6; C04B040/00D4
 AT 229487
                 IPCI C04B0040-00 [ICM, 7]; C04B0022-08 [ICS, 7]; C04B0022-14
                          [ICS, 7]; C04B0022-00 [ICS, 7, C*]
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TPCR
                        C04B0022-00 [I,C*]; C04B0022-08 [I,A]; C04B0022-14
                        [I,A]; C04B0040-00 [I,A]; C04B0040-00 [I,C*]
                 ECLA
                        C04B022/08; C04B022/14G6; C04B040/00D4
 ES 2186289
                 IPCI
                        C04B0040-00 [ICM, 7]; C04B0022-08 [ICS, 7]; C04B0022-14
                        [ICS, 7]; C04B0022-00 [ICS, 7, C*]
                 IPCR
                        C04B0022-00 [I,C*]; C04B0022-06 [I,A]; C04B0022-08
                        [I,A]; C04B0022-14 [I,A]; C04B0024-00 [I,C*];
                        C04B0024-02 [I,A]; C04B0024-06 [I,A]; C04B0024-10
                        [I,A]; C04B0024-12 [I,A]; C04B0024-26 [I,A];
                        C04B0024-28 [I.A]; C04B0024-32 [I.A]; C04B0028-00
                        [I,C*]; C04B0028-02 [I,A]; C04B0040-00 [I,C*];
                        C04B0040-00 [I,A]; C04B0103-12 [N,A]; C04B0103-14 [N,A]
                 ECLA
                        C04B022/08; C04B022/14G6; C04B040/00D4
CA 2324393
                 IPCI
                        C04B0022-08 [ICM, 7]; C04B0022-00 [ICM, 7, C*];
                        C04B0024-02 [ICS, 7]; C04B0024-00 [ICS, 7, C*]
                 TPCR
                        C04B0022-00 [I,C*]; C04B0022-06 [I,A]; C04B0022-08
                        [I,A]; C04B0022-14 [I,A]; C04B0024-00 [I,C*];
                        C04B0024-02 [I,A]; C04B0024-06 [I,A]; C04B0024-10
                        [I,A]; C04B0024-12 [I,A]; C04B0024-26 [I,A];
                        C04B0024-28 [I,A]; C04B0024-32 [I,A]; C04B0028-00
                        [I,C*]; C04B0028-02 [I,A]; C04B0040-00 [I,C*];
                        C04B0040-00 [I,A]; C04B0103-12 [N,A]; C04B0103-14 [N,A]
                 ECLA
                        C04B022/08; C04B022/14G6; C04B040/00D4
US 6514327
                 IPCI
                        C04B0022-08 | ICM, 71; C04B0022-00 | ICM, 7, C*1;
                        C04B0024-12 [ICS, 7]; C04B0024-00 [ICS, 7, C*];
                        C23F0011-00 [ICS, 7]
                 TPCR
                        C04B0022-00 [I,C*]; C04B0022-06 [I,A]; C04B0022-08
                        [I,A]; C04B0022-14 [I,A]; C04B0024-00 [I,C*];
                        C04B0024-02 [I,A]; C04B0024-06 [I,A]; C04B0024-10
                        [I,A]; C04B0024-12 [I,A]; C04B0024-26 [I,A];
                        C04B0024-28 [I,A]; C04B0024-32 [I,A]; C04B0028-00
                        [I,C*]; C04B0028-02 [I,A]; C04B0040-00 [I,C*];
                        C04B0040-00 [I,A]; C04B0103-12 [N,A]; C04B0103-14 [N,A]
                 NCL.
                        106/014.110; 106/014.050; 106/014.150; 106/014.440;
                        106/287.170; 106/724.000; 106/727.000; 106/728.000;
                        106/802.000; 106/808.000; 106/810.000; 106/823.000
                 ECLA
                        C04B022/08; C04B022/14G6; C04B040/00D4
JP 2001180994
                 IPCI
                        C04B0022-08 [I,A]; C04B0022-14 [I,A]; C04B0022-00
                        [I,C*]; C04B0024-02 [I,A]; C04B0024-06 [I,A];
                        C04B0024-10 [I,A]; C04B0024-12 [I,A]; C04B0024-26
                        [I,A]; C04B0024-28 [I,A]; C04B0024-32 [I,A];
                        C04B0024-00 [I,C*]; C04B0028-02 [I,A]; C04B0028-00
                        [I.C*]
                 IPCR
                        C04B0022-00 [I,C*]; C04B0022-06 [I,A]; C04B0022-08
                        [I,A]; C04B0022-14 [I,A]; C04B0024-00 [I,C*];
                        C04B0024-02 [I,A]; C04B0024-06 [I,A]; C04B0024-10
                        [I,A]; C04B0024-12 [I,A]; C04B0024-26 [I,A];
                        C04B0024-28 [I,A]; C04B0024-32 [I,A]; C04B0028-00
                        [I,C*]; C04B0028-02 [I,A]; C04B0040-00 [I,C*];
                        C04B0040-00 [I,A]; C04B0103-12 [N,A]; C04B0103-14 [N,A]
AU 2001038785
                 IPCI
                        C04B0022-00 [ICM, 7]; C04B0022-14 [ICS, 7]; C04B0024-04
                        [ICS, 7]; C04B0024-00 [ICS, 7]
                        C04B0022-00 [I,C*]; C04B0024-00 [I,C*]; C04B0022-00
                 IPCR
                        [I,A]; C04B0022-14 [I,A]; C04B0024-00 [I,A];
                        C04B0024-04 [I.A]
NZ 511309
                 IPCI
                        C04B0022-00 [ICM, 7]; C04B0022-14 [ICS, 7]; C04B0024-00
                        [ICS, 7]; C04B0024-04 [ICS, 7]
                 TPCR
                        C04B0022-00 [I,C*]; C04B0022-00 [I,A]; C04B0022-14
                        [I,A]; C04B0024-00 [I,C*]; C04B0024-00 [I,A];
                        C04B0024-04 [I,A]
                      C04B0022-08 [ICM, 7]; C04B0022-00 [ICM, 7, C*]
 IN 2001MA00353 IPCI
AB The setting accelerator compns. comprise ≥1 an alkali-free and
```

```
Cl-free aluminum salt including ≥1 a complex binder for Al ion and
≥1 a corrosion inhibitor. The aluminum salt is selected from
aluminum sulfate, nitrate, glycolate, lactate, acetate, formate,
hydroxy-formate, or mixts. thereof. The complex binder is
selected from nitrilotriacetic acid, ethylenediamine tetra-acetic acid,
gluconic acid, heptonic acid, phosphonic acid or mixts. thereof. The
corrosion inhibitor is selected from alkyne, butindiol, propargylalc.,
3-(methylamino)propylamine, 3-(Dimethylamino)propylamine,
3-(Diethylamino) propylamine, Cyclohexylamine, N-Methylcyclohexylamine,
N-Ethylcyclohexylamine, 1-(Dimethylamino)-2-propanol,
1-(Ethylamino)-2-propanol, 1-(Cyclohexylamino)-2-propanol,
3-Amino-1-propanol, 2-Aminoethanol, 2,2'-Iminodiethanol,
2-(Methylamino)ethanol, 2-(Dimethylamino)ethanol,
2-(Ethylamino)ethanol, and 2-(Diethylamino)ethanol. A thickening agent
selected from bentonite, bentone, biopolymers, alginate, polyglycolether,
acrylate-based or urethane-based thickener, carboxylic acid ester, or
mixts. thereof may be also added to the compns. in the from of aqueous solution
The resulting accelerators are suitable for cement-based mortars,
concrete, plasters, and shotcrete.
concrete mortar plaster setting accelerator corrosion inhibitor
Setting agents
   (accelerators, based on Al salt; low viscosity, Cl-free stabilized
   hardening accelerators of concrete and mortar)
Concrete modifiers
   (accelerators; low viscosity, C1-free stabilized hardening accelerators
   of concrete and mortar)
Alkynes
RL: MOA (Modifier or additive use); USES (Uses)
   (corrosion inhibitor; low viscosity, Cl-free stabilized hardening
   accelerators of concrete and mortar)
Carboxylic acids, uses
RL: MOA (Modifier or additive use); USES (Uses)
   (esters, thickening agent; low viscosity, Cl-free stabilized hardening
   accelerators of concrete and mortar)
Corrosion inhibitors
   (of cement concrete and mortar; low viscosity, Cl-free stabilized
   hardening accelerators of concrete and mortar)
Glycols, uses
RL: MOA (Modifier or additive use); USES (Uses)
   (polyglycolether, thickening agent; low viscosity, Cl-free stabilized
   hardening accelerators of concrete and mortar)
Cement (construction material)
   (portland; low viscosity, Cl-free stabilized hardening accelerators of
   concrete and mortar)
Plaster
   (setting accelerator for; low viscosity, C1-free stabilized hardening
   accelerators of concrete and mortar)
Mortar
   (shotcrete, setting accelerator for; low viscosity, Cl-free stabilized
   hardening accelerators of concrete and mortar)
Bentonite, uses
Biopolymers
Urethanes
RL: MOA (Modifier or additive use); USES (Uses)
   (thickening agent; low viscosity, C1-free stabilized hardening
   accelerators of concrete and mortar)
60-00-4, Ethylenediamine tetraacetic acid, uses
                                                 139-13-9,
Nitrilotriacetic acid
                       526-95-4, Gluconic acid 2782-86-7, Heptonic acid
13598-36-2, Phosphonic acid
RL: MOA (Modifier or additive use); USES (Uses)
   (accelerator binder; low viscosity, C1-free stabilized hardening
   accelerators of concrete and mortar)
```

ST

ΤТ

ΙT

```
100-37-8, 2-(Diethylamino)ethanol 100-60-7, N-Methylcyclohexylamine
     103-00-4, 1-(Cyclohexylamino)-2-propanol
                                                104-78-9,
                                   107-19-7, Propargylalcohol 108-01-0, 2-(
     3-(Diethylamino)propylamine
     Dimethylamino)ethanol 108-16-7,
     1-(Dimethylamino)-2-propanol
                                   108-91-8, Cyclohexylamine, uses
                                                                       109-55-7,
     3-(Dimethylamino)propylamine 109-83-1, 2-(Methylamino)ethanol
     110-73-6, 2-(Ethylamino)ethanol 111-42-2, 2,2'-Iminodiethanol, uses
     141-43-5, 2-Aminoethanol, uses 156-87-6, 3-Amino-1-propanol
     N-Ethylcyclohexylamine 6291-84-5, 3-(Methylamino)propylamine
     11070-67-0, Butynediol 40171-86-6, 1-(Ethylamino)-2-propanol
     RL: MOA (Modifier or additive use); USES (Uses)
        (corrosion inhibitor; low viscosity, Cl-free stabilized hardening
        accelerators of concrete and mortar)
     139-12-8, Aluminum acetate 7360-53-4, Aluminum formate
     10043-01-3, Aluminum sulfate 13473-90-0, Aluminum nitrate
                                                                    18917-91-4,
     Aluminum lactate 19878-87-6, Aluminum glycolate
     RL: MOA (Modifier or additive use); USES (Uses)
        (setting accelerator; low viscosity, Cl-free stabilized hardening
        accelerators of concrete and mortar)
IT
     1340-68-7, Bentone 9005-32-7, Alginic acid
                                                    10344-93-1, Acrylate, uses
     RL: MOA (Modifier or additive use); USES (Uses)
        (thickening agent; low viscosity, Cl-free stabilized hardening
        accelerators of concrete and mortar)
RE.CNT 7
             THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD
(1) Lunkenheimer, R; WO 9818740 A 1998 CAPLUS
(2) Mbt Holding Ag; EP 0812812 A 1997 CAPLUS
(3) Nordhausen Schachtbau; DD 266344 A 1989 CAPLUS
(4) Sika Ag; EP 0076927 A 1983 CAPLUS
(5) Sika Aq; EP 0657398 A 1995 CAPLUS
(6) Stepita; CS 217017 A 1985 CAPLUS
(7) United States Gypsum Co; GB 2140794 A 1984 CAPLUS
L9
    ANSWER 24 OF 55 CAPLUS COPYRIGHT 2009 ACS on STN
     2001:317316 CAPLUS
AN
DN
    135:77844
ED
     Entered STN: 04 May 2001
ΤI
     Effects of thiazolium counter anion and reaction media on the activity of
     immobilized thiazolium catalyst
AU
    Tajima, Hideo; Niitsu, Takashi; Inoue, Hakuai; Ito, Masato M.
     Department of Bioengineering, Soka University, Hachioji, 192-8577, Japan
CS
SO
    Journal of Chemical Engineering of Japan (2001), 34(4), 553-557
    CODEN: JCEJAO: ISSN: 0021-9592
PB
    Society of Chemical Engineers, Japan
DT
    Journal
LA
    English
CC
    38-3 (Plastics Fabrication and Uses)
     Section cross-reference(s): 22, 33, 35
ΔR
    We quant. studied the effects of counter anions and solvents on the
     catalytic activity of thiazolium due to the completion of the formose
     reaction using the highly active immobilized catalyst. The relation
     between counter anions and the catalytic activity of thiazolium was
     represented very well by the electron donor constant and the basic constant of
    the anions. The solvent effect was represented by the individual solvent parameter. In this study, it was given an important information about the
     effects of the counter anion and the solvent on the reaction using an
     immobilized thiazolium catalyst.
    immobilized thiazolium bound copolymer catalyst; counter anion immobilized
     thiazolium catalyst activity; reaction media immobilized thiazolium
     catalyst activity; solvent effect immobilized thiazolium catalyst
    activity; formose reaction immobilized thiazolium catalyst activity
```

ΙT

Catalysts

Counterions Solvent effect (effects of thiazolium counter anion and reaction media on activity of copolymer immobilized thiazolium catalyst) 71-47-6, Formate, uses 71-50-1, Acetate, uses 302-04-5. Thiocyanate, uses 14797-55-8, Nitrate, uses 14797-73-0, Perchlorate 14996-02-2, Sulfate (HSO41-), uses 16053-58-0, Methanesulfonate anion 16887-00-6, Chloride, uses 16984-48-8, Fluoride, uses Iodide, uses 24959-67-9, Bromide, uses 52912-48-8 RL: NUU (Other use, unclassified); USES (Uses) (counter ion; effects of thiazolium counter anion and reaction media on activity of copolymer immobilized thiazolium catalyst) 137-00-8D, 2-(4-Methyl-5-thiazolyl)ethanol, reaction products with chloromethylated divinylbenzene-styrene copolymer 9003-70-7D, Divinylbenzene-styrene copolymer, chloromethylated, thiazolium derivative RL: CAT (Catalyst use); USES (Uses) (effects of thiazolium counter anion and reaction media on activity of copolymer immobilized thiazolium catalyst) 50-00-0, Formaldehyde, reactions 108-01-0, 2-Dimethylaminoethanol 8069-42-9, Formose RL: RCT (Reactant); RACT (Reactant or reagent) (effects of thiazolium counter anion and reaction media on activity of copolymer immobilized thiazolium catalyst) 64-17-5, Ethanol, uses 67-56-1, Methanol, uses 67-68-5, DMSO, uses 68-12-2, DMF, uses 75-05-8, Acetonitrile, uses 107-12-0, Ethyl cyanide 110-86-1, Pyridine, uses 123-91-1, Dioxane, uses 141-78-6, Ethyl acetate, uses 7732-18-5, Water, uses RL: NUU (Other use, unclassified); USES (Uses) (solvent; effects of thiazolium counter anion and reaction media on activity of copolymer immobilized thiazolium catalyst) RE.CNT 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD (1) Bassedas, M; Reactive Polymers 1987, V6, P109 CAPLUS (2) Chang, B; J Chinese Chem Soc 1983, V30, P55 CAPLUS (3) Chastrette, M; Can J Chem 1985, V63, P3492 CAPLUS (4) Edwards, J; J Am Chem Soc 1954, V76, P1540 CAPLUS (5) El Hange Chahire, J; J Am Chem Soc 1983, V105, P2335 (6) El Hange Chahire, J; J Chem Soc Perkin Trans II 1989, P25 (7) Isaacs, N; Physical Organic Chemistry 1987 (8) Matsumoto, T; J Am Chem Soc 1984, V106, P4829 CAPLUS (9) Nipponkagakukai; Kagakubinran Kisohen II in Japanese 1984 (10) Ruasse, M; Pure Appl Chem 1997, V69, P1923 CAPLUS (11) Saimoto, H; Tetrahedron Lett 1989, V30, P2553 CAPLUS (12) Tajima, H; J Chem Eng Japan 1999, V32, P776 CAPLUS (13) Tajima, H; J Chem Eng Japan 2000, V33, P793 CAPLUS (14) Tee, O; J Org Chem 1986, V51, P2150 CAPLUS (15) Van den Berg, H; J Mol Catal 1989, V51, P13 CAPLUS L9 ANSWER 25 OF 55 CAPLUS COPYRIGHT 2009 ACS on STN AN 1999:728127 CAPLUS DN 131:338432 ED Entered STN: 17 Nov 1999 Aqueous ink for ink-jet printing Aoyama, Tetsuya IN PA Seiko Epson Corp., Japan Jpn. Kokai Tokkyo Koho, 12 pp. CODEN: JKXXAF Patent LA Japanese TC ICM C09D011-00

42-12 (Coatings, Inks, and Related Products)

FAN.CNT 1

PATENT NO. KIND DATE APPLICATION NO. DATE JP 1315229 A 1999116 JP 1998-123755 19980506 PRAI JP 1998-123755 19980506 CLASS PATENT NO. CLASS PATENT FAMILY CLASSIFICATION CODES JP 11315229 ICM C09D011-00 [ICM,6]										
PI JP 11315229 A 19991116 JP 1998-123755 19980506 PRRAI JP 1998-123755 19980506 CLASS PATENT NO. CLASS PATENT FAMILY CLASSIFICATION CODES JP 11315229 ICM C09D011-00 [ICM,6] IPCI C09D0011-00 [ICM,6] IPCI C09D0011-00 [I,A]; C09D0011-00 [I,C*] AB Title ink comprises at least (A) aqueous pigment, (B) water, (C) water-soluble cationic polymer, and (D) carboxyl-containing organic acid/salt. Thus, 100 g of an ink (pH value 9.7) was prepared by dissolving 5 g of pigment (Direct Black 32) in 50 g ultrapure water, adding 1.5 g polyallylamine (Mw = 2000), 0.5 g acetic acid, and more ultrapure water, and then filtrating with a metal-mesh filter, showing good storage stability, printing glossiness, and ink-jet head reliability, and water resistance of images. ST aq jet ink storage stability; polyallylamine aq jet ink printing glossiness water resistance; acetic acid head reliability ink jet printing IT Inks (jet-printing; preparation of aqueous ink for ink-jet printing) T50-00-0DP, Formalin, reaction products with polyallylamine and formic acid 64-18-6DP, Formic acid, reaction products with formic acid and formalin 3051-89-4P, Polyallylamine, reaction products with formic acid and formalin 3051-89-4P, Polyallylamine, RL: IMF (Industrial manufacture); POF (Polymer in formulation); PRP (Properties); IEM (Technical or engineered material use); PREP										
JP 11315229 ICM C09D011-00 [ICM,6]	PRAI	JP 11315229 JP 1998-123		A 19	9991116					
JP 11315229 ICM C09D011-00 [ICM,6] IPCI C09D0011-00 [ICM,6] IPCR C09D0011-00 [ICM,6] Title ink comprises at least (A) aqueous pigment, (B) water, (C) water-soluble cationic polymer, and (D) carboxyl-containing organic acid/salt. Thus, 100 g of an ink (pH value 9.7) was prepared by dissolving 5 g of pigment (Direct Black 32) in 50 g ultrapure water, adding 1.5 g polyallylamine (Nw = 2000), 0.5 g acetic acid, and more ultrapure water, and then filtrating with a metal-mesh filter, showing good storage stability, printing glossiness, and ink-jet head reliability, and water resistance of images. ST aq jet ink storage stability; polyallylamine aq jet ink printing glossiness water resistance; acetic acid head reliability ink jet printing Inks (jet-printing; preparation of aqueous ink for ink-jet printing) 50-00-0DP, Formalin, reaction products with polyallylamine and formic acid 64-18-6DP, Formal acid, reaction products with polyallylamine, reaction products with formic acid and formalin 30551-89-4P, Polyallylamine RL: INF (Industrial manufacture); POF (Polymer in formulation); PRP (Properties); IEM (Technical or engineered material use); PREP										
AB Title ink comprises at least (A) aqueous pigment, (B) water, (C) water-soluble cationic polymer, and (D) carboxyl-containing organic acid/salt. Thus, 100 g of an ink (pH value 9.7) was prepared by dissolving 5 g of pigment (Direct Black 32) in 50 g ultrapure water, adding 1.5 g polyallylamine (Mw = 2000), 0.5 g acetic acid, and more ultrapure water, and then filtrating with a metal-mesh filter, showing good storage stability, printing glossiness, and ink-jet head reliability, and water resistance of images. ag jet ink storage stability; polyallylamine and jet ink printing Inks II Inks (jet-printing; preparation of aqueous ink for ink-jet printing) 50-00-0DP, Formalin, reaction products with polyallylamine and formic acid 64-18-6DP, Formic acid, reaction products with polyallylamine, reaction products with formic acid and formalin 3051-89-4DP, Polyallylamine, Polyallylamine RL: IMF (Industrial manufacture); POF (Polymer in formulation); PRP (Properties); IEM (Technical or engineered material use); PREP			ICM CO	C09D011-00 C09D0011-00 [ICM,6]						
an ink (pH value 9.7) was prepared by dissolving 5 g of pigment (Direct Black 32) in 50 g ultrapure water, adding 1.5 g polyallylamine (Mw = 2000), 0.5 g acetic acid, and more ultrapure water, and then filtrating with a metal-mesh filter, showing good storage stability, printing glossiness, and ink-jet head reliability, and water resistance of images. ST aq jet ink storage stability; polyallylamine aq jet ink printing glossiness water resistance; acetic acid head reliability ink jet printing IT Inks (jet-printing; preparation of aqueous ink for ink-jet printing) ST 50-00-0DP, Formalin, reaction products with polyallylamine and formic acid 6+18-6DP, Formic acid, reaction products with polyallylamine and formalin, uses 30551-89-4DP, Polyallylamine, reaction products with formic acid and formalin 30551-89-4P, Polyallylamine RL: IMF (Industrial manufacture); POF (Polymer in formulation); PRP (Properties); TEM (Technical or engineered material use); PREP			omprises a	at least	(A) aqueou	s pigment, (B) water,				
(Properties); TEM (Technical or engineered material use); PREP	ST	an ink (pH value 9.7) was prepared by dissolving 5 g of pigment (Direct Black 32) in 50 g ultrapure water, adding 1.5 g polyallylamine (Mw = 2000), 0.5 g acetic acid, and more ultrapure water, and then filtrating with a metal-mesh filter, showing good storage stability, printing glossiness, and ink-jet head reliability, and water resistance of images. as jet ink storage stability; polyallylamine agiet ink printing glossiness water resistance; acetic acid head reliability ink jet printing Inks (jet-printing; preparation of aqueous ink for ink-jet printing) 55 -00-0DP, Formalin, reaction products with polyallylamine and formic acid 64-18-6DP, Fornic acid, reaction products with polyallylamine and formalin, uses 30551-89-4DP, Polyallylamine, reaction products with formic acid and formalin 30551-89-4P,								
(Preparation); USES (Uses) (ink containing; preparation of aqueous ink for ink-jet printing) IT 50-21-5, uses 56-81-5, 1,2,3-Propanetriol, uses 57-11-4, Octadecanoic	IT	inting)								

acid, uses 64-19-7, Acetic acid, uses 65-85-0, Benzoic acid, uses 69-72-7, uses 72-17-3, Sodium lactate 79-09-4, Propionic acid, uses 108-01-0, 2-(Dimethylamino)ethanol 111-48-8 112-34-5, Diethylene glycol monobutyl ether 141-53-7, Sodium 585-88-6, Maltitol 1310-58-3, Potassium hydroxide, uses 9014-85-1, Surfynol 465 14307-43-8, Ammonium tartrate, uses 51807-73-9, Propylamine acetate RL: MOA (Modifier or additive use); USES (Uses) (ink containing; preparation of aqueous ink for ink-jet printing) ΙT 9002-98-6, SP 012 26470-16-6, PAS H 5L 26590-05-6, PAS J 81

32698-04-7, PAS A 1 71550-12-4, Danfix 723 RL: POF (Polymer in formulation); PRP (Properties); TEM (Technical or engineered material use); USES (Uses)

(ink containing; preparation of aqueous ink for ink-jet printing) 61-73-4, C.I. Basic Blue 9 1330-38-7, Direct Blue 86 2580-78-1,

Reactive Blue 19 2783-94-0, C.I. Food Yellow 3 3214-47-9, Direct 5001-72-9, Direct Red 31 6428-38-2, Direct Black Yellow 50 3875-70-5 32 8005-03-6, C.I. Acid Black 2 12224-98-5, C.I. Pigment Red 81 15876-56-9, Solvent Yellow 15

RL: TEM (Technical or engineered material use); USES (Uses)

(pigment, ink containing; preparation of aqueous ink for ink-jet printing)

- ANSWER 26 OF 55 CAPLUS COPYRIGHT 2009 ACS on STN L9
- AN 1999:219915 CAPLUS
- DN 130:249136
- ED Entered STN: 08 Apr 1999
 - Amino acid sequencing of proteins or peptides from the carboxy terminus using an acid anhydride to generate oxazolone derivatives
- TN Tsugita, Akira; Takamoto, Keiji; Ataka, Tatsuaki; Sakuhara, Toshihiko; Uchida, Toyoaki

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PA Seiko Instruments Inc., Japan
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Eur. Pat. Appl., 72 pp. SO CODEN: EPXXDW

Patent DT

English T.A.

ICM G01N033-68 IC

ICS C07K001-12

9-16 (Biochemical Methods) Section cross-reference(s): 34

FAN.CNT 1

	PA:	TENT :	NO.		KIN)	DATE			APPL	ICAT	ION I	NO.		D.	ATE	
						-									-		
PI	EP	9055	19		A1		1999	0331		EP 1	997-	3069	36		1	99709	908
	EP	9055	19		B1		2005	0525									
		R:					ES,	FR,	GB,	GR,	ΙT,	LI,	LU,	NL,	SE,	MC,	PT,
				LT,													

PRAI EP 1997-306 CLASS	936	19970908
PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
EP 905519	ICM	G01N033-68
	ICS	C07K001-12
	IPCI	G01N0033-68 [ICM,6]; C07K0001-12 [ICS,6]; C07K0001-00 [ICS,6,C*]
	IPCR	C07K0001-00 [I,C*]; C07K0001-12 [I,A]; G01N0033-68
		[I,C*]; G01N0033-68 [I,A]
	ECLA	C07K001/12; G01N033/68A4B

In a C-terminal amino acid sequencing method, a carboxy-terminal amino acid of a protein or a peptide is liberated by reacting the protein or peptide with an acid anhydride to convert the carboxy terminal amino acid residue into an oxazolone derivative and releasing the derivatized amino acid residue with an acid and alc., the released amino acid is isolated and identified, and the steps are repeated. The method was tested using the peptide Leu-Trp-Met-Arg-Phe, acetic anhydride in the presence of acetic acid, and pentafluoropropionic acid and methanol or heptafluorobutyric acid and ethanol. HPLC and mass spectrometry were used in the anal.

carboxy terminal protein sequencing acid anhydride oxazolone

IT Alcohols, uses

RL: NUU (Other use, unclassified); USES (Uses)

(acid and, in release of derivatized amino acid; carboxy terminus amino acid sequencing of proteins or peptides using acid anhydrides to generate oxazolone derivs.)

Acids, uses

RL: NUU (Other use, unclassified); USES (Uses)

(alcs. and, in release of derivatized amino acid; carboxy terminus amino acid sequencing of proteins or peptides using acid anhydrides to generate oxazolone derivs.)

HPLC

Mass spectrometry

Protein sequence analysis

(carboxy terminus amino acid sequencing of proteins or peptides using acid anhydrides to generate oxazolone derivs.)

Anhvdrides

RL: NUU (Other use, unclassified); RCT (Reactant); RACT (Reactant or reagent); USES (Uses)

(carboxy terminus amino acid sequencing of proteins or peptides using acid anhydrides to generate oxazolone derivs.)

Peptides, reactions

RL: PRP (Properties); RCT (Reactant); RACT (Reactant or reagent) (carboxy terminus amino acid sequencing of proteins or peptides using acid anhydrides to generate oxazolone derivs.)

Proteins, general, reactions

RL: PRP (Properties); RCT (Reactant); RACT (Reactant or reagent) (carboxy terminus amino acid sequencing of proteins or peptides using acid anhydrides to generate oxazolone derivs.)

IT Amines, uses

Esters, uses

RL: NUU (Other use, unclassified); USES (Uses)

(in release of derivatized amino acid; carboxy terminus amino acid sequencing of proteins or peptides using acid anhydrides to generate oxazolone derivs.)

IT 64-17-5, Ethanol, uses

RL: NUU (Other use, unclassified); USES (Uses)

(acid and, in release of derivatized amino acid; carboxy terminus amino acid sequencing of proteins or peptides using acid anhydrides to generate oxazolone derivs.)

IT 67-56-1, Methanol, reactions

RL: NUU (Other use, unclassified); RCT (Reactant); RACT (Reactant or reagent); USES (Uses)

(acid and, in release of derivatized amino acid; carboxy terminus amino acid sequencing of proteins or peptides using acid anhydrides to generate oxazolone derivs.)

IT 64-18-6D, Formic acid, halogenated, esters, reactions 108-24-7

RL: NUU (Other use, unclassified); RCT (Reactant); RACT (Reactant or reagent); USES (Uses)

(carboxy terminus amino acid sequencing of proteins or peptides using acid anhydrides to generate oxazolone derivs.)

IT 16305-75-2 67201-39-2 216297-50-6

RL: PRP (Properties); RCT (Reactant); RACT (Reactant or reagent) (carboxy terminus amino acid sequencing of proteins or peptides using acid anhydrides to generate oxazolone derivs.)

IT 375-22-4, Heptafluorobutyric acid

RL: NUU (Other use, unclassified); USES (Uses)

(ethanol and, in release of derivatized amino acid; carboxy terminus amino acid sequencing of proteins or peptides using acid anhydrides to generate oxazolone derivs.)

T 221676-64-8

RL: FMU (Formation, unclassified); PRP (Properties); FORM (Formation, nonpreparative)

(formation of; carboxy terminus amino acid sequencing of proteins or peptides using acid anhydrides to generate oxazolone derivs.)

T 64-19-7, Acetic acid, uses

RL: NUU (Other use, unclassified); USES (Uses)

(in presence of; carboxy terminus amino acid sequencing of proteins or peptides using acid anhydrides to generate oxazolone derivs.)

IT 7732-18-5, Water, uses

RL: NUU (Other use, unclassified); USES (Uses)

(in release of derivatized amino acid; carboxy terminus amino acid sequencing of proteins or peptides using acid anhydrides to generate oxazolone derive.)

IT 108-01-0, 2-Dimethylaminoethanol

RL: PRP (Properties); RCT (Reactant); RACT (Reactant or reagent) (in release of derivatized amino acid; carboxy terminus amino acid sequencing of proteins or peptides using acid anhydrides to generate oxazolone derivs.)

IT 422-64-0, Pentafluoropropionic acid

RL: NUU (Other use, unclassified); RCT (Reactant); RACT (Reactant or reagent); USES (Uses)

(methanol and, in release of derivatized amino acid; carboxy terminus amino acid sequencing of proteins or peptides using acid anhydrides to generate oxazolone derivs.)

IT 378-75-6P, Methylpentafluoropropionate

RL: NUU (Other use, unclassified); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(preparation of, for use in release of derivatized amino acid; carboxy terminus amino acid sequencing of proteins or peptides using acid anhydrides to generate oxazolone derivs.)

THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD RE CNT 7 RE

- (1) Bailey, M; US 5180807 A CAPLUS
- (2) Bailey, M; TECH PROTEIN CHEM 3, PAP ANNU SYMP PROTEIN SOC 1992, V5TH, P12
- (3) Basu, G; BIOPOLYMERS 1991, V31(14), P1763 CAPLUS
- (4) Boyd, L; US 5468843 A CAPLUS
- (5) Boyd, L: WO 9503066 A CAPLUS
- (6) Kurabo Ind; JP 06027113 A CAPLUS
- (7) Kurabo Ind; JP 06027113 A 1994 CAPLUS
- ANSWER 27 OF 55 CAPLUS COPYRIGHT 2009 ACS on STN
- AN 1998:351635 CAPLUS DN
- 129:101910
- OREF 129:20837a,20840a
- ED Entered STN: 10 Jun 1998
- TΙ Electrostatographic toner and two component electrophotographic developer
- IN Miyajima, Koichiro; Fujimori, Yoshihisa
- Toyo Ink Mfg. Co., Ltd., Japan PA SO Jpn. Kokai Tokkvo Koho, 7 pp.
- CODEN: JKXXAF
- DT Patent
- Japanese LA
- ICM G03G009-08 TC:
 - ICS G03G009-087; G03G015-08
 - 74-3 (Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes)

FAN.CNT 1

PATENT NO.		KIND	DATE	APPLICATION NO.	DATE
PI JP 1014896: PRAI JP 1996-30	A	19980602 19961118	JP 1996-306044	19961118	
CLASS					
PATENT NO.	CLASS	PATENT	FAMILY CLAS	SIFICATION CODES	
JP 10148962	ICM ICS IPCI IPCR	G03G000	0-087; G03G0 09-08 [ICM,6	15-08]; G03G0009-087 [ICS,6] : G03G0009-08 [I.A]; G0	

G03G0015-08 [I.A] AB The electrostatog, toner comprises a coloring resin containing a colorant and a binder, and fine powder having a smaller average diameter than the coloring resin's, wherein the fine powder is prepared by a multi-step soap-free polymerization and has 3.6-6.8 pH. An alkylacrylate and/or an

[I,C*]; G03G0009-087 [I,A]; G03G0015-08 [I,C*];

alkvlmethacrvlate

are polymerized or copolymd. before the last polymerization step and a polymerizable

carboxylic acid or a polymerizable carboxylic acid salt is polymerized in the last polymerization step. The toner provides the stable charge for long time under different environments and especially the charge-up prevention at low temperature to eliminate the decrease of the image contrast and the fogging.

- electrostatog toner electrophotog developer fine powder
- Electrophotographic toners
 - (two-component developer toners; toner and two component electrophotog. developer)
- 9011-14-7P, Poly(methylmethacrylate) 25322-25-2P, Acrylic acid-methylmethacrylate copolymer 26950-79-8P, Methacrylic acid-methylmethacrylate copolymer sodium salt

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RL: PNU (Preparation, unclassified); TEM (Technical or engineered material
     use); PREP (Preparation); USES (Uses)
        (fine powder for electrostatog, toner)
     64-18-6, Formic acid, uses 79-10-7, Acrylic acid, uses
     RL: TEM (Technical or engineered material use); USES (Uses)
       (fine powder for electrostatog. toner)
     108-01-0, Dimethylaminoethanol 142-72-3, Magnesium acetate
     557-34-6, Zinc acetate 2638-94-0, Azobiscyanovaleric acid
     RL: TEM (Technical or engineered material use); USES (Uses)
       (toner and two component electrophotog, developer)
    ANSWER 28 OF 55 CAPLUS COPYRIGHT 2009 ACS on STN
    1997:502724 CAPLUS
DN 127:163170
OREF 127:31615a,31618a
ED Entered STN: 09 Aug 1997
TI Coating methods without intermediate compositions on electrodeposited
    substrates
    Horibe, Kyoichi; Haneishi, Hidehiko; Mitsuji, Masaru; Yabuta, Motoshi;
    Okumura, Yasumasa
    Kansai Paint Co., Ltd., Japan
    Eur. Pat. Appl., 35 pp.
    CODEN: EPXXDW
    Patent
     English
     ICM B05D007-00
     ICS C09D005-44; C08G018-10
     42-2 (Coatings, Inks, and Related Products)
    Section cross-reference(s): 55
FAN.CNT 1
    PATENT NO.
                      KIND DATE
                                                               DATE
                                         APPLICATION NO.
                       -----
    EP 785034
                       A1 19970723 EP 1997-100801
                                                              19970120
    EP 785034
                       B1 20021106
       R: DE, GB
                      A 19970729
B2 20060712
A 19980526
     JP 09192588
                             19970729 JP 1996-26244
                                                                19960122
     JP 3796286
US 5756221
CA 2195607
PRAI JP 1996-26244
                       A 19980526 US 1997-785600
A1 19970723 CA 1997-2195607
                                                               19970117
                       A
                              19960122
CLASS
PATENT NO. CLASS PATENT FAMILY CLASSIFICATION CODES
EP 785034
               ICM B05D007-00
                ICS
                      C09D005-44; C08G018-10
                IPCI B05D0007-00 [ICM,6]; C09D0005-44 [ICS,6]; C08G0018-10
                      [ICS,6]; C08G0018-00 [ICS,6,C*]
                IPCR B05D0001-36 [I,C*]; B05D0001-36 [I,A]; B05D0003-02
                       [I,C*]; B05D0003-02 [I,A]; B05D0003-10 [I,C*];
                       B05D0003-10 [I,A]; B05D0005-00 [I,C*]; B05D0005-00
                       [I,A]; B05D0007-00 [I,C*]; B05D0007-00 [I,A];
                       B05D0007-24 [I,C*]; B05D0007-24 [I,A]; C08G0018-00
                       [I,C*]; C08G0018-58 [I,A]; C09D0005-44 [I,C*];
                       C09D0005-44 [I,A]
                ECLA
                      B05D007/00N3C6; C08G018/58; C08G018/58F; C09D005/44E
JP 09192588
                IPCI
                      B05D0001-36 [I,A]; B05D0007-24 [I,A]; C09D0005-44 [I,A]
                TPCR
                      B05D0001-36 [I,C*]; B05D0001-36 [I,A]; B05D0003-02
                       [I,C*]; B05D0003-02 [I,A]; B05D0003-10 [I,C*];
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B05D0003-10 [I,A]; B05D0005-00 [I,C*]; B05D0005-00 [I,A]; B05D0007-00 [I,C*]; B05D0007-00 [I,A]; B05D0007-24 [I,C*]; B05D0007-24 [I,A]; C08G0018-00 [I,C*]; C08G0018-58 [I,A]; C09D0005-44 [I,C*];

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TC:

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C09D0005-44 [I,A]
                ECLA
                       B05D007/00N3C6; C08G018/58; C08G018/58F; C09D005/44E
US 5756221
                IPCI
                       C25D0013-06 [ICM, 6]; C25D0013-04 [ICM, 6, C*]
                       B05D0001-36 [I,C*]; B05D0001-36 [I,A]; B05D0003-02
                IPCR
                       [I,C*]; B05D0003-02 [I,A]; B05D0003-10 [I,C*];
                       B05D0003-10 [I,A]; B05D0005-00 [I,C*]; B05D0005-00
                       [I,A]; B05D0007-00 [I,C*]; B05D0007-00 [I,A];
                       B05D0007-24 [I,C*]; B05D0007-24 [I,A]; C08G0018-00
                       [I,C*]; C08G0018-58 [I,A]; C09D0005-44 [I,C*];
                       C09D0005-44 [I.A]
                       428/626.000; 204/488.000; 204/501.000; 428/416.000
                NCL
                ECLA
                       B05D007/00N3C6; C08G018/58; C08G018/58F; C09D005/44E
CA 2195607
                IPCI
                       C09D0005-44 [ICM,6]; C25D0013-00 [ICS,6]
                IPCR
                       B05D0001-36 [I,C*]; B05D0001-36 [I,A]; B05D0003-02
                       [I,C*]; B05D0003-02 [I,A]; B05D0003-10 [I,C*];
                       B05D0003-10 [I,A]; B05D0005-00 [I,C*]; B05D0005-00
                       [I,A]; B05D0007-00 [I,C*]; B05D0007-00 [I,A];
                       B05D0007-24 [I,C*]; B05D0007-24 [I,A]; C08G0018-00
                       [I,C*]; C08G0018-58 [I,A]; C09D0005-44 [I,C*];
                       C09D0005-44 [I,A]
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AB Automotive coating films having superior finish appearance, corrosion resistance, weatherability, chipping resistance, acid resistance, abrasion resistance, etc., are formed simply. The coating method comprises applying, onto a substrate, a cationic electrodepostable coating composition comprising (A) a polyurethane-modified epoxy resin-amine adduct, obtained by a reaction of (A-I) a polyurethane compound having 1 terminal isocyanate group, obtained by a reaction of (a) a polyurethane compound having a number-average

mol. weight 50-8000, (b) a polyisocyanate compound, and (c) a compound having 1 active H atom; (A-2) a bisphenol-type epoxy resin having ≥2 epoxy groups; and (A-3) an active-H-containing amine compound, and (B) a nonionic film-forming resin, at weight ratio (A)/(B) (15-95): (5-85) and the coating composition comprising substantially no pigment, then heat-curing the formed electrocoating film, and applying an aqueous coating composition comprising a metallic pigment and/or a coloring pigment and a high-solid-content coating composition comprising (C) a carboxyl group-containing compound, (D) a vinvi

type polymer containing an epoxy group, a hydroxyl group and a hydrolyzable alkoxysilyl group, (E) a reactive organopolysiloxane, and (F) crosslinked polymer fine particles, but comprising substantially no pigment, by 2-coat 2-bake or by 2-coat 1-bake process. A In phosphated Fe plate was first electrodeposited with a composition containing the adduct of isophorone diisocyanate-Placcel 208 prepolymer with bisphenol A diglycidyl ether polymer 52, Bu methacrylate-hydroxyethyl methacrylate-FM-3X-styrene copolymer 23, blocked isocyanate crosslinker 25, polypropylene glycol 1 g, formic acid, Pb acetate, Pb silicate, Bu2SnO, C, TiO2, and surfactant as an emulsion, and cured to give an electrocoated plate. Over the electrocoated plate was coated aqueous base coat containing acrylic acid-Bu acrylate-2-hydroxyethyl methacrylate-Me methacrylate-styrene copolymer dimethylaminoethanol salt solution 40, Bu acrylate-2-ethylhexyl acrylate-2-hydroxyethyl acrylate-methacrylic acid-Me methacrylate-styrene copolymer dimethylaminoethanol salt solution 275, amino resin crosslinker 25, Al paste 20, and solvent 273 parts and a high-solid-content acrylic top coat containing hexahydrophthalic anhydride-3-methyl-1,5-pentanediol-trimethylolpropane copolymer, Bu acrylate-glycidyl methacrylate-4-hydroxybutyl acrylate-3-methacryloxypropyltrimethoxysilane-styrene copolymer, X41-1067 reactive siloxane, and crosslinked beads in a 2-coat-2-bake (80, 150°) process to give a finish coat having good surface appearance and weatherability. ST automotive coating film; two coat bake process automotive coating;

polyurethane electrocoating two coat bake process; ag pigmented base coat

automotive coating; high solid top coat automotive coating

T Polysiloxanes, uses

RL: TEM (Technical or engineered material use); USES (Uses)
(Me methoxy, glycidyl group-containing, in high-solid-content acrylic top
coat; in manufacture of weatherable automotive coating finish using two coat
bake process over electrocoated metal substrate)

IT Polyesters, uses

RL: PEP (Physical, engineering or chemical process); PRP (Properties); TEM (Technical or engineered material use); PROC (Process); USES (Uses) (acrylic, high-solid-content top coat; in manufacture of weatherable

automotive coating finish using two coat bake process over electrocoated metal substrate)

IT Polyurethanes, preparation

Polyurethanes, preparation

RL: IMF (Industrial manufacture); PEP (Physical, engineering or chemical process); PREP (Preparation); PROC (Process)

(epoxy, electrocoat; in manufacture of weatherable automotive coating finish using two coat bake process over electrocoated metal substrate)

IT Polyoxyalkylenes, uses

RL: PEP (Physical, engineering or chemical process); TEM (Technical or engineered material use); PROC (Process); USES (Uses)

(in electrocoat; in manufacture of weatherable automotive coating finish using two coat bake process over electrocoated metal substrate)

IT Epoxy resins, preparation

Epoxy resins, preparation

RL: IMF (Industrial manufacture); PEP (Physical, engineering or chemical process); PREP (Preparation); PROC (Process)

(polyurethane-, electrocoat; in manufacture of weatherable automotive coating finish using two coat bake process over electrocoated metal substrate)

IT Coating process

(two-layer-one-bake; in manufacture of weatherable automotive coating finish using two coat bake process over electrocoated metal substrate)

IT 72065-17-9 193608-46-7

RI: PEP (Physical, engineering or chemical process); PRP (Properties); TEM (Technical or engineered material use); PROC (Process); USES (Uses) (aqueous pigmented base coat; in manufacture of weatherable automotive

(aqueous pigmented base coat; in manufacture of weatherable automotive coating

finish using two coat bake process over electrocoated metal substrate)
1 2008-99-8DP, Bisphenol A diglycidyl ether polymer, reaction product with
polyurethane 112363-56-1P 146115-98-2DP, reaction product with epoxy
resin

RI: IMF (Industrial manufacture); PEP (Physical, engineering or chemical process); PREP (Preparation); PROC (Process)

(electrocoat; in manufacture of weatherable automotive coating finish using two coat bake process over electrocoated metal substrate)

IT 25322-69-4, Polypropylene glycol

RL: PEP (Physical, engineering or chemical process); TEM (Technical or engineered material use); PROC (Process); USES (Uses)

(in electrocoat; in manufacture of weatherable automotive coating finish using two coat bake process over electrocoated metal substrate)

IT 191171-40-1 193608-50-3

RL: PEP (Physical, engineering or chemical process); PRP (Properties); TEM (Technical or engineered material use); PROC (Process); USES (Uses)

(in high-solid-content acrylic top coat; in manufacture of weatherable automotive coating finish using two coat bake process over electrocoated metal substrate)

L9 ANSWER 29 OF 55 CAPLUS COPYRIGHT 2009 ACS on STN

AN 1995:995041 CAPLUS

DN 124:117073

OREF 124:21805a,21808a

- ED Entered STN: 22 Dec 1995
- ΤI Preparation and formulation of N-benzylaminoacyl-4-phenoxyazetidinones for treatment of lung disease (cystic fibrosis).
- IN Davies, Philip
- PA Merck and Co., Inc., USA
- SO PCT Int. Appl., 97 pp. CODEN: PIXXD2
- DT Patent
- English
- LA ICM A61K038-00 ΙĊ
- ICS A61K031-395
- 27-5 (Heterocyclic Compounds (One Hetero Atom))

CC 27-5 (Heterocyclic Compounds (One Hetero Atom)) Section cross-reference(s): 1, 63								
FAN.CNT 1 PATENT NO.		KIND	DATE	APPLICATION NO.	DATE			
KZ,	AU, BB, LK, LR,	A1 BG, BR,	19950914 BY, CA, CN, MD, MG, MN,	WO 1995-US2938 CZ, EE, FI, GE, MX, NO, NZ, PL,	19950307 HU, JP, KG, KR,			
RW: KE, LU, SN,	MW, SD,	SZ, UG, PT, SE,	AT, BE, CH, BF, BJ, CF,	DE, DK, ES, FR, CG, CI, CM, GA,	GN, ML, MR, NE,			
CA 2184385 AU 9520994 AU 686780 EP 755262		A B2 A1	19950925 19980212 19970129	CA 1995-2184385 AU 1995-20994 EP 1995-913618	19950307 19950307			
R: AT, JP 09510212 PRAI US 1994-2124 WO 1995-US29	20	T A	19971014	GR, IE, IT, LI, JP 1995-523641	LU, NL, PT, SE 19950307			
CLASS PATENT NO.	CLASS I	PATENT F	AMILY CLASSI	FICATION CODES				
WO 9524207	ICM 11CS 11IPCI	A61K038- A61K031- A61K031- C07D0205; [I,C*]; A61K0031 [I,A]; A61K0038 [I,C*]; A61K0038 [I,C*]; A61P0001 [I,C*]; A61P0001 [I,A]; A61P0011 [I,A]; A61P0011 [I,A];	-00	A61K0031-395 [IC CO700205-08 [J,A] [I,A]; A61K0031- A61K0031-40 [I,C*]; A61K0031- A61K0031-445 [I,C [I,C*]; A61K0031- A61K0038-00 [I,A]; [I,A]; A61P0009- G1P0095-00 [I,C*]; I,C*]; A61P0031-C A61P0033-02 [I,A]; G17A]; A61P0031-C A61P0033-02 [I,A]; G700405-00 [I,C*]	25,6] 1, A61K0031-395 -397 [1,C*]; 1, A61K0031-40 -4427 [1,A]; -4495 [1,A]; 1, A61K0038-17 00 [1,C*]; -A61F0011-00 00 [1,C*]; 1, A61F0019-00 4 [1,A]; 1, C0700401-00 00 [1,C*];			
CA 2184385	IPCI I	C07D0205 [I,C*]; A61K0031 [I,A]; A A61K0031 [I,A]; A	8-16 [ICM,6]; 6-00 [I,C*]; A61K0031-395 8-397 [I,A]; A61K0031-4427 8-443 [I,A]; A61K0031-495	A61K0031-395 [IC C07D0205-08 [I,A] [I,A]; A61K0031- A61K0031-40 [I,C*]; A61K0033 A61K0031-445 [I,C*]; A61K0031- A61K0038-00 [I,A]	; A61K0031-395 -397 [I,C*]; 1]; A61K0031-40 L-4427 [I,A]; -41; A61K0031-445 495 [I,A];			

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[I,C*]; A61K0038-17 [I,A]; A61P0009-00 [I,C*];
A61P0009-08 [I,A]; A61P0009-10 [I,A]; A61P0011-00
[I,C*]; A61P0011-00 [I,A]; A61P0011-10 [I,A];
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C07D0403-12 [I,A]; C07D0405-00 [I,C*]; C07D0405-06
[I, A]
A61K0038-00 [ICM,6]; A61K0031-395 [ICS,6]
C07D0205-00 [I,C*]; C07D0205-08 [I,A]; A61K0031-395
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A61P0011-14 [I,A]; A61P0029-00 [I,C*]; A61P0029-00
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A61P0033-00 [I,C*]; A61P0033-02 [I,A]; C07D0401-00
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C07D0403-12 [I.Al; C07D0405-00 [I.C*]; C07D0405-06
[I.Al
A61K038/17A2+M
A61K0038-00 [ICM,6]; A61K0031-395 [ICS,6]
C07D0205-00 [I,C*]; C07D0205-08 [I,A]; A61K0031-395
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[I,A]; A61K0031-4427 [I,C*]; A61K0031-4427 [I,A];
A61K0031-443 [I,A]; A61K0031-445 [I,C*]; A61K0031-445
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A61P0009-08 [I,A]; A61P0009-10 [I,A]; A61P0011-00
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A61P0011-14 [I,A]; A61P0029-00 [I,C*]; A61P0029-00
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A61P0033-00 [I,C*]; A61P0033-02 [I,A]; C07D0401-00
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C07D0403-12 [I.Al; C07D0405-00 [I.C*]; C07D0405-06
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C07D0401-12 [ICS,6]; C07D0401-00 [ICS,6,C*];
C07D0403-12 [ICS,6]; C07D0403-00 [ICS,6,C*];
C07D0405-06 [ICS,6]; C07D0405-00 [ICS,6,C*]
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[I,C*]; A61K0031-395 [I,A]; A61K0031-397 [I,C*];
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A61K0031-443 [I,A]; A61K0031-445 [I,C*]; A61K0031-445
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[I,C*]; A61P0011-00 [I,A]; A61P0011-10 [I,A];
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A61P0011-14 [I,A]; A61P0029-00 [I,C*]; A61P0029-00

AU 9520994

EP 755262

JP 09510212

IPCI

IPCR

ECLA

IPCI

IPCR

ECLA

TPCT

IPCR

S MARPAT 124:117073

AB A pharmaceutical composition comprising a therapeutically effective, nontoxic amount of an (F)-actin shortening protein, a therapeutically effective amount of an elastase inhibitor, and a pharmaceutically acceptable carrier is claimed. More specifically, the protein is gelsolin and the elastase inhibitor is a title compound [I; R = alkyl, R = alkyl, alkoxyalkyl; M = H, alkyl, hydroxyalkyl, haloalkyl, alkenyl, alkoxyalkyl; Ra, Rb = H; R2, R3 = H, alkyl, halo, alkoxy; R2R3 = atoms to form a methylenedioxy group, furan ring; R4 = QCOYNR7R8; Q = bond; Y = NR9(CHR12)nCR10R11; R9-R12 = H, alkyl; R7, R8 = H, alkyl, alkoxyalkyl, hydroxyalkyl; n = 1-5; R89 = atoms to form a mono- or disubstituted heterocycle]. Compns. containing [S-(R*,S*)]-2-[4-[(4-methyl)piperazin-1-yl]carbonyl]phenoxy]-3, 3-diethyl-N-[1-(3,4-methylenedioxyphenyl)butyl]-4-oxo-1-azetidinecarboxamide are claimed, as is a method for treating a patient with lung disease with the claimed compns. with amts. sufficient to return lung function to 75-90% of

normal as measured by FEV1.

ST benzylaminoacylphenoxyazetidinone prepn lung disease treatment; sputum viscosity redn benzylaminoacylphenoxyazetidinone gelsolin; cystic fibrosis treatment benzylaminoacylphenoxyazetidinone gelsolin

IT Cystic fibrosis Lung, disease

(treatment; preparation and formulation of

Ι

N-benzylaminoacy1-4-phenoxyazetidinones with gelsolin for treatment of lung disease)

T Proteins, specific or class

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(gelsolins, preparation and formulation of

N-benzylaminoacyl-4-phenoxyazetidinones with gelsolin for treatment of lung disease)

IT 9004-06-2, Elastase

RL: BSU (Biological study, unclassified); MSC (Miscellaneous); BIOL (Biological study)

(inhibitors; preparation and formulation of

N-benzylaminoacyl-4-phenoxyazetidinones with gelsolin for treatment of lung disease)

IT 157341-09-8P 157341-10-1P 157341-11-2P 157341-12-3P 157341-13-4P

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157341-14-5P
                 157341-15-6P
                                157341-16-7P 157341-17-8P
                                                            157341-18-9P
    157341-19-0P 157341-20-3P
                                157341-21-4P 157341-22-5P
                                                            157341-23-6P
    157341-24-7P 157341-25-8P
                                157341-26-9P 157341-27-0P
                                                            157341-28-1P
    157341-29-2P 157341-30-5P
                                157341-31-6P 157341-32-7P
                                                            157341-34-9P
    157341-40-7P 157341-41-8P
                                157341-43-0P 157341-44-1P
                                                            157341-45-2P
    157341-46-3P 157341-48-5P
                                157343-04-9P 157343-05-0P 157343-06-1P
    157343-08-3P 157343-09-4P
                                157343-10-7P 157343-11-8P 157343-14-1P
    157343-15-2P 157343-16-3P 157343-18-5P 157343-19-6P 157343-20-9P
    157343-21-0P 157343-22-1P 157343-23-2P 157343-24-3P 157343-25-4P
    157343-26-5P 157343-27-6P 157343-28-7P 157343-29-8P 157343-30-1P
    157343-34-5P 157343-35-6P 157343-36-7P 157343-37-8P 157343-38-9P
    157343-39-0P 157343-40-3P 157343-41-4P 157343-42-5P 157343-43-6P
    157343-44-7P 157343-45-8P 157343-47-0P 157343-48-1P 157343-49-2P
    157343-50-5P 157343-52-7P 157343-53-8P 157343-54-9P
                                                            157343-55-0P
    157343-56-1P 157343-57-2P 157343-58-3P 157343-59-4P
                                                            157343-60-7P
    157343-61-8P 157343-62-9P 157343-63-0P 157343-64-1P 157343-65-2P
    157343-66-3P 157343-68-5P 157343-69-6P 157343-70-9P 157343-72-1P
    157343-73-2P 157343-74-3P 157343-76-5P 157343-77-6P 157343-78-7P
    157343-80-1P 157381-58-3P 157382-05-3P 157385-25-6P 159120-97-5P
    172900-37-7P
                  172900-38-8P 172900-39-9P 172900-40-2P
                                                            172900-41-3P
                  172900-43-5P 172900-44-6P
                                             172900-45-7P
                                                            172900-46-8P
    172900-42-4P
                 172900-49-1P 173007-16-4P 173007-17-5P
    172900-48-0P
    RL: BAC (Biological activity or effector, except adverse); BSU (Biological
    study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);
    BIOL (Biological study); PREP (Preparation); USES (Uses)
       (preparation and formulation of N-benzylaminoacyl-4-phenoxyazetidinones with
       gelsolin for treatment of lung disease)
    100-46-9, Benzylamine, reactions 102-11-4,
    N-Benzyl-N, N'-dimethylethylenediamine 103-76-4,
    N-(2-Hydroxyethyl)piperazine 107-14-2, Chloroacetonitrile
                                                              108-00-9,
    N,N-Dimethylethylenediamine 108-01-0, N,N-Dimethylaminoethanol
    109-01-3, N-Methylpiperazine 109-89-7, Diethylamine, reactions
    109-94-4, Ethyl formate 111-42-2, Diethanolamine, reactions
    123-75-1, Pyrrolidine, reactions 142-25-6,
    N,N,N'-Trimethylethylenediamine 500-22-1, Pyridine-3-carboxaldehyde
    505-66-8, Homopiperazine 3099-31-8, 3-Picolyl chloride 5292-43-3,
    tert-Butyl bromoacetate 6404-31-5 27578-60-5,
    1-(2-Aminoethyl)piperidine 31166-44-6, N-Benzyloxycarbonylpiperazine
    41324-66-7, Proline benzyl ester 56777-24-3, Benzyl L-lactate
    57260-71-6, N-tert-Butoxycarbonylpiperazine 127063-07-4 139256-79-4
    157341-52-1 172900-50-4 172900-51-5 172900-52-6 172900-53-7
    RL: RCT (Reactant); RACT (Reactant or reagent)
       (preparation and formulation of N-benzylaminoacyl-4-phenoxyazetidinones with
       gelsolin for treatment of lung disease)
    26331-21-5P
                 51388-00-2P 54714-50-0P 90727-50-7P 118808-13-2P
    136470-00-3P
                  144243-45-8P 157341-38-3P 157341-39-4P 157341-50-9P
    172900-47-9P
    RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
    (Reactant or reagent)
       (preparation and formulation of N-benzylaminoacyl-4-phenoxyazetidinones with
       gelsolin for treatment of lung disease)
RE.CNT 4
             THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD
(1) Anon: EP 0337549 A1 CAPLUS
(2) Anon: EP 0481671 A1 CAPLUS
(3) Anon; US 5260224 A CAPLUS
(4) Anon; US 5276139 A CAPLUS
    ANSWER 30 OF 55 CAPLUS COPYRIGHT 2009 ACS on STN
   1994:482440 CAPLUS
   121:82440
OREF 121:14797a,14800a
```

RE

1.9

AN

DN

- ED Entered STN: 20 Aug 1994 Kinetics and products of the gas-phase reactions of 03 with amines and related compounds AII Tuazon, E.C.; Atkinson, R.; Aschmann, S.M.; Arey, J. CS Statewide Air Pollut, Res. Cent., Univ. California, Riverside, CA, 92521, Research on Chemical Intermediates (1994), 20(3-5), 303-20 SO CODEN: RCINEE; ISSN: 0922-6168 Journal LA English CC 22-13 (Physical Organic Chemistry) Section cross-reference(s): 59 AB The kinetics and products of the gas-phase reactions of 03 with a series of aliphatic amines and related compds. have been investigated at 298 ± 2 K and 740 Torr total pressure of air. The absolute rate consts. obtained (in cm3 mol.-1 s-1 units) were: methylamine, (7.4 ± 2.4) + 10-21; dimethylamine, $(1.67 \pm 0.20) + 10-18$; trimethylamine, $(7.84 \pm$ 0.87) + 10-18; 2-(dimethylamino)ethanol, (6.76 \pm 0.83) + 10-18; and tetramethylhydrazine, (5.21 \pm 0.60) + 10-18. The major products observed from the O3 reactions with the use of in situ FT-IR absorption spectroscopy were: from trimethylamine, (CH3) 2NCHO, CH3N: CH2 and HCHO; and from dimethylamine, CH3N: CH2, CH3NO2, and HCHO. Possible reaction mechanisms are presented and discussed. ozone reaction amine kinetics mechanism Kinetics, reaction Reaction mechanism (of ozone with amines and related compds.) Amines, reactions RL: RCT (Reactant); RACT (Reactant or reagent) (reaction of, and of related compds., with ozone, kinetics and mechanism of) 50-00-0P, Formaldehyde, preparation 51-80-9P, N, N, N', N'-Tetramethyldiaminomethane 64-18-6P, Formic acid, preparation 68-12-2P, DMF, preparation 75-52-5P, Nitromethane, preparation 123-39-7P, N-Methylformamide 124-38-9P, Carbon dioxide, preparation 1761-67-7P, N-Methylmethylenimine 7732-18-5P, Water, preparation RL: FORM (Formation, nonpreparative); PREP (Preparation) (formation of, in reaction of ozone with amine in gas phase) 10028-15-6, Ozone, reactions RL: RCT (Reactant); RACT (Reactant or reagent) (reaction of, with aliphatic amines and related compds. in gas phase, kinetics and mechanism of) 74-89-5, Methylamine, reactions 6415-12-9, Tetramethylhydrazine RL: RCT (Reactant); RACT (Reactant or reagent) (reaction of, with ozone in gas phase, kinetics of) 75-50-3, Trimethylamine, reactions 108-01-0, 2-(Dimethylamino) 124-40-3, Dimethylamine, reactions ethanol RL: RCT (Reactant); RACT (Reactant or reagent) (reaction of, with ozone in gas phase, kinetics of and product study of) ANSWER 31 OF 55 CAPLUS COPYRIGHT 2009 ACS on STN L9 AN 1990:58331 CAPLUS DN 112:58331 OREF 112:10013a, 10016a ED Entered STN: 17 Feb 1990 Cationic electrodeposition coating materials containing aprotic onium salts
- Iwazawa, Naozumi; Isozaki, Osamu PA Kansai Paint Co., Ltd., Japan

TN

SO Jpn. Kokai Tokkyo Koho, 12 pp. CODEN: JKXXAF

Patent DT LA Japanese

ICM C09D005-44 TC

ICS C09D003-48; C09D005-44; C25D013-06

42-7 (Coatings, Inks, and Related Products)

Section cross-reference(s): 55

FAN.CNT 1

KIND DATE APPLICATION NO. PATENT NO. ----19890720 JP 1988-3645 PI JP 01182376 A 19880111 PRAI JP 1988-3645 19880111

CLASS

PATENT NO. CLASS PATENT FAMILY CLASSIFICATION CODES

JP 01182376 TCM

C09D005-44 TCS C09D003-48; C09D005-44; C25D013-06

IPCI C09D0005-44 [ICM, 4]; C09D0003-48 [ICS, 4]; C09D0005-44 [ICS, 4]; C25D0013-06 [ICS, 4]; C25D0013-04 [ICS, 4, C*]

AB Coating materials curable at low temperature and forming thick coatings contain resins having α, β-unsatd. carbonvl groups and primary or secondary OH groups and aprotic onium group -CHR2CH2W+ -O2CR1 (R1 = OH, alkoxy, ester, C1-8 hydrocarbyl groups optionally substituted with halogens, or H; R2 = H, OH, C1-8 hydrocarbyl groups; W+ = Z+R3R4R5 or

Y+R3R4; Z = N or P; Y = S; R3, R4, and R5 = C1-14 organic group, heterocyclic ring member. Thus, styrene 20, 2-hydroxyethyl methacrylate 10, Bu acrylate 35, glycidyl methacrylate 35, tert-Bu peroxyoctoate 3 parts were

mixed, added during 3 h to 60 parts HOCH2CH2OBu at 110°, aged 7 h at 110°, cooled to 250°, mixed with 10.5 parts

diethanolamine, heated 2 h at 50-70°, mixed with acrylic acid 10.5, hydroquinone 0.02, and Et4NBr 0.1 part and heated 4 h at 110° to

prepare a resin solution This solution (100 parts) was mixed with rutile 20,

talc 10, and PhCH2OH 1 part, ball-milled, mixed with a 186:89:90.1 2-ethylhexyl glycidyl ether-dimethylaminoethanol-lactic acid reaction product (I) 10, AcOH 2.5, and H2O 475 parts, electrodeposited on phosphated steel,

and baked at 120° to form a coating. hydroxyvinyl polymer electrodeposition; cationic electrodeposition coating material; aprotic onium salt electrodeposition coating; ammonium salt

electrodeposition coating Phosphonium compounds

Quaternary ammonium compounds, uses and miscellaneous

Sulfonium compounds RL: USES (Uses)

(hydroxyvinyl polymers containing, for cationic electrodeposition coating materials)

Coating materials (cationic, electrodeposited, hydroxyvinyl polymers, containing aprotic

ammonium salts) Epoxides

RL: USES (Uses)

(reaction products, with amines and carboxylic acids, in cationic electrodeposition coating materials containing hydroxyvinyl polymers)

Carboxylic acids, compounds

RL: USES (Uses)

(reaction products, with amines and epoxy resins, in cationic electrodeposition coating materials containing hydroxyvinyl polymers)

Amines, compounds RL: USES (Uses)

(reaction products, with carboxylic acids and epoxy resins, in cationic electrodeposition coating materials containing hydroxyvinyl polymers) 79-10-7D, 2-Propenoic acid, reaction products with dibutylamine and epoxy

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resin 108-18-9D, Diisopropylamine, reactions with acrylic and epoxy
resin and hydroxyethyl acrylate-isophorone diisocyanate adduct
111-42-2D, reaction products with acrylic acid and epoxy resin
111-92-2D, Dibutylamine, reaction products with acrylic acid and epoxy
      25068-38-6D, EPIKOTE 1004, reaction products with acrylic acid and
diethanolamine 69645-73-4, Acrylic acid-butyl acrylate-glycidyl
methacrylate-2-hydroxyethyl methacrylate-methyl methacrylate copolymer
78724-20-6D, reaction products with acrylic acid and diisopropanolamine
and epoxy resin 84778-06-3D, EPIKOTE 152, reaction products with acrylic
acid and dibutylamine 124996-28-7
RL: USES (Uses)
```

(cationic electrodeposition coatings, containing aprotic onium salts)

50-21-5D, Lactic acid, reaction products with dimethylaminoethanol and ethylhexyl glycidyl ether 64-18-6D, Formic acid, reaction products with butylene oxide and methyldiethanolamine 64-19-7D, Acetic acid, reaction products with butylene oxide and triethylamine 102-71-6D, Triethanolamine, reaction products with acetic acid and butylene oxide 105-59-9D, reaction products with butylene oxide and formic acid 108-01-0D, reaction products with ethylhexyl glycidyl ether and lactic acid 111-48-8D, β-Thiodiglycol, reaction products with acrylic acid and epoxy resin 603-35-0D, reaction products with acetic acid and epoxy resin 2461-15-6D, 2-Ethylhexyl glycidyl ether, reaction products with dimethylaminoethanol and lactic acid 26249-20-7D, Butylene oxide, reaction products with formic acid and methyldiethanolamine 125062-24-0D, reaction products with dimethylaminoethanol and acetic acid RL: USES (Uses)

(cationic electrodeposition coatings, containing hydroxyvinyl polymers)

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T. 9
    ANSWER 32 OF 55 CAPLUS COPYRIGHT 2009 ACS on STN
ΔN
    1990:22477 CAPLUS
DN
    112:22477
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OREF 112:3933a,3936a

ED Entered STN: 21 Jan 1990

Curable cationic polymer compositions for coatings IN Isozaki, Osamu; Iwasawa, Naozumi

PA Kansai Paint Co., Ltd., Japan

SO Ger. Offen., 11 pp. CODEN: GWXXBX

DT Patent

LA German

IC ICM C08L101-00

ICS C08L033-04; C08L061-04; C08L063-10; C08L067-06; C08L075-04; C08J003-24

ICA C08L101-06; C08L033-14

CC 42-10 (Coatings, Inks, and Related Products)

FAN.CNT 1				
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI DE 3841413	A1	19890622	DE 1988-3841413	19881208
DE 3841413	C2	19920430		
JP 01152110	A	19890614	JP 1987-311652	19871208
JP 2612457	B2	19970521		
JP 01152117	A	19890614	JP 1987-311653	19871208
CA 1338575	С	19960903	CA 1988-584748	19881201
GB 2213488	A	19890816	GB 1988-28256	19881202
GB 2213488	В	19911127		
PRAI JP 1987-311652	A	19871208		
JP 1987-311653	A	19871208		
CLASS				

PATENT NO. CLASS PATENT FAMILY CLASSIFICATION CODES

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DE 3841413
                 TCM
                        C08L101-00
                 TCS
                        C08L033-04; C08L061-04; C08L063-10; C08L067-06;
                        C08L075-04; C08J003-24
                 TCA
                        C08L101-06; C08L033-14
                 IPCI
                        C08L0101-00 [ICM, 4]; C08L0033-04 [ICS, 4]; C08L0061-04
                        [ICS, 4]; C08L0061-00 [ICS, 4, C*]; C08L0063-10 [ICS, 4];
                        C08L0063-00 [ICS, 4, C*]; C08L0067-06 [ICS, 4];
                        C08L0067-00 [ICS, 4, C*]; C08L0075-04 [ICS, 4];
                        C08L0075-00 [ICS, 4, C*]; C08J0003-24 [ICS, 4];
                        C08L0101-06 [ICA, 4]; C08L0033-14 [ICA, 4]; C08L0033-00
                        [ICA, 4, C*]
                 IPCR
                        C08F0290-00 [I,C*]; C08F0290-14 [I,A]; C08F0299-00
                        [I,C*]; C08F0299-02 [I,A]; C08J0003-24 [I,C*];
                        C08J0003-24 [I,A]
                        C08F290/14; C08F299/02; C08J003/24H
                 ECLA
 JP 01152110
                 TPCT
                        C08F0008-00 [ICM, 4]; C08F0004-00 [ICS, 4]; C08F0008-30
                        [ICS, 4]; C08F0008-34 [ICS, 4]; C08F0008-40 [ICS, 4];
                        C08F0299-00 [ICS, 4]; C08J0005-00 [ICS, 4]
                 IPCR
                        C08F0004-00 [I,C*]; C08F0004-00 [I,A]; C08F0008-00
                        [I,C*]; C08F0008-00 [I,A]; C08F0008-30 [I,A];
                        C08F0008-34 [I,A]; C08F0008-40 [I,A]; C08F0290-00
                        [I,C*]; C08F0290-00 [I,A]; C08F0299-00 [I,C*];
                        C08F0299-00 [I,A]; C08G0059-00 [I,C*]; C08G0059-00
                        [I.A]; C08G0059-17 [I.A]; C08G0063-00 [I.C*];
                        C08G0063-68 [I,A]; C08G0063-91 [I,A]; C08J0005-00
                        [T.C*1: C08J0005-00 [T.A]
JP 01152117
                 TPCT
                        C08F0299-00 [ICM, 4]; C08F0004-00 [ICS, 4]; C08J0005-00
                        [ICS, 4]
                 IPCR
                        C08F0004-00 [I,C*]; C08F0004-00 [I,A]; C08F0290-00
                        [I,C*]; C08F0290-00 [I,A]; C08F0299-00 [I,C*];
                        C08F0299-00 [I,A]; C08J0005-00 [I,C*]; C08J0005-00
                        [I,A]; C09D0163-10 [I,C*]; C09D0163-10 [I,A];
                        C09D0167-06 [I,C*]; C09D0167-07 [I,A]; C09D0175-14
                        [I,C*]; C09D0175-14 [I,A]; C09D0175-16 [I,A]
CA 1338575
                 IPCI
                        C08F0002-50 [ICM,6]; C08F0002-46 [ICM,6,C*]
                 IPCR
                        C08F0290-00 [I,C*]; C08F0290-14 [I,A]; C08F0299-00
                        [I,C*]; C08F0299-02 [I,A]; C08J0003-24 [I,C*];
                        C08J0003-24 [I,A]
GB 2213488
                 IPCI
                        C08F0008-00 [ICM, 4]; C08G0059-14 [ICS, 4]; C08G0059-17
                        [ICS, 4]; C08G0059-20 [ICS, 4]; C08G0059-00 [ICS, 4, C*];
                        C08F0008-30 [ICA, 4]; C08F0008-34 [ICA, 4]; C08F0008-40
                        [ICA, 41
                 IPCR
                        C08F0290-00 [I,C*]; C08F0290-14 [I,A]; C08F0299-00
                        [I.C*]; C08F0299-02 [I,A]; C08J0003-24 [I,C*];
                        C08J0003-24 [I,A]
AB
    Storage-stable, curable compns. giving water-resistant cured coatings
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- AB Storage-stable, curable compans giving water-resistant cured coatings contain polymers bearing polymerizable unsatn. and polymers (which may be the same or different) bearing sulfonium, phosphonium, or quaternary ammonium carboxylate groups. Heating an epoxy resin (Epikote 154) 209, acrylic acid 84, 2,2"-thiodiethanol 31, hydroquinone 0.3, and BuOCHZCH2OH 139 parts at 80° for 3 h gave a 70% solution (Gardner viscosity Z at 25°) of polymer with peak mol. weight 1000, unsatd. group content 3.6 mol/kg, and onium salt content 0.77 mol/kg. Coating this solution (100 µm) on glass or steel and baking 10 min at 120° gave a film with acetone insoly. 89.9% (40°, 8 h) and good water resistance (40°, 7 days).
- ST onium carboxylate polymer coating; sulfonium carboxylate polymer coating; epoxy resin sulfonium deriv coating; thiodiethanol adduct epoxy coating; acrylic acid adduct coating; water resistance coating; solvent resistance coating
- IT Phosphonium compounds Quaternary ammonium compounds, polymers

Sulfonium compounds RL: USES (Uses) (polymers, coatings containing unsatd, polymers and, storage-stable, manufacture of) Coating materials (water-resistant, onium salt polymers and unsatd. polymers as) 26007-17-0P 92880-74-5P, Epikote 154 acrylate 124181-01-7P 124363-46-8P RL: PREP (Preparation) (coatings containing polymeric onium carboxylates and, storage-stable, manufacture of) IT 75-98-9DP, Pivalic acid, reaction products with epoxy resins and pyridine 25068-38-6DP, reaction products with pivalic acid and pyridine RL: PREP (Preparation) (coatings containing unsatd. polymers and, storage-stable, manufacture of) 64-18-6DP, Formic acid, salts with unsatd. quaternary ammonium TТ polymers 106-89-8DP, reaction products with poly(ethylene itaconate) and pyridine, formate salt 108-01-0DP, reaction products with glycidyl methacrylate copolymer and acetic acid 110-86-1DP, Pyridine, reaction products with epichlorohydrin and poly(ethylene itaconate), formate salt 111-48-8DP, 2,2'-Thiodiethanol, reaction products with Epikote 154 acrylate and acrylic acid 26007-17-0DP, Ethylene glycol-itaconic acid copolymer, reaction products with epichlorohydrin and pyridine, formate salt 92880-74-5DP, Epikote 154 acrylate, onium salt derivs., carboxylate salts 124274-17-5P 124363-46-8DP, reaction products with (dimethylamino)ethanol and acetic acid RL: TEM (Technical or engineered material use); PREP (Preparation); USES (Uses) (coatings, storage-stable, manufacture of) RE.CNT THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD RE (1) Anon; US 4338232 A CAPLUS (2) Anon; US 4857566 A CAPLUS L9 ANSWER 33 OF 55 CAPLUS COPYRIGHT 2009 ACS on STN AN 1987:139229 CAPLUS DN 106:139229 OREF 106:22731a,22734a ED Entered STN: 01 May 1987 ΤI Effect of crosslink density and content of urethane groups in polymer matrix on physicomechanical properties of polyurethane foams ΑU Zeltina, D.; Gruzins, I.; Zeltins, V.; Alksnis, A.; Zhmud, N. P.; Karlivans, V. CS Inst. Khim. Drev., Riga, USSR SO Latvijas PSR Zinatnu Akademijas Vestis, Kimijas Serija (1987), (1), 85-9 CODEN: LZAKAM: ISSN: 0002-3248 DT Journal LA Russian 37-6 (Plastics Manufacture and Processing) AB The physicochem. properties of polyurethane (PU) foams, based on polvisocvanate B and Rianol (glycerol-oxalic acid copolymers), were studied as a function of crosslink d. and urethane group content (c) of the PU matrix. The softening temperature (Ts) and compressive strength (GC) of foams increased with increasing crosslink d. for PU with c ≤5.25 mequiv/g and decreased with increasing crosslink d. for PU with c >5.25 mequiv/g due to partial thermal degradation of the PU matrix during foam preparation. The increase of pH of PU foams after hydrolytic aging in 1:1 glycerol-H2O mixture was due to the decrease in concentration of hydrolytically unstable methylene formate side groups in the

polymer matrix. The high pH of PU foams after hydrolytic aging decreased

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the corrosion of metals thermally insulated with PU foams.
     polyurethane foam property crosslink density
    Urethane polymers, properties
     RL: PRP (Properties)
        (cellular, physicomech. properties of Rianol, effects of crosslink d.
        and urethane group content on)
     Crosslinking
        (d., of polyurethane foams, physicomech. properties in relation to)
     Siloxanes and Silicones, uses and miscellaneous
     RL: USES (Uses)
        (foam regulators, for polyurethane foams)
     Blowing agents
        (trichlorotrifluoroethane, for polyurethane foams)
ΤТ
     76-13-1, Freon 113
     RL: USES (Uses)
        (blowing agent, for polyurethane foams)
     56-81-5D, polymers with oxalic acid and polyisocyanates 75-13-8D,
     Isocyanic acid, esters, polymers with glycerol and oxalic acid
     144-62-7D, polymers with glycerol and polyisocyanates
     RL: USES (Uses)
       (cellular, physicomech. properties of Rianol, effects of crosslink d.
        and urethane group content on)
     108-01-0, 2-(Dimethylamino)ethanol
                                         115-96-8
     2641-56-7
     RL: USES (Uses)
        (polyurethane foam containing, physicomech. properties of)
    ANSWER 34 OF 55 CAPLUS COPYRIGHT 2009 ACS on STN
L9
AN
    1983:454575 CAPLUS
DN
    99:54575
OREF 99:8534h,8535a
ED
    Entered STN: 12 May 1984
    Acrylate-modified melamine resin which is stable on storage and its use
    Adam, Wilhelm; Wagner, Curt A.; Konrad, Renate; Engelhardt, Friedrich;
TN
    Riegel, Ulrich; Eckhardt, Georg W.; Piesch, Steffen
PA
    Cassella A.-G., Fed. Rep. Ger.
SO
    U.S., 7 pp. Cont.-in-part of U.S. Ser. No. 185,165, abandoned.
    CODEN: USXXAM
DT
    Patent
LA
   English
    C08L061-28; C08L061-32
TC
INCL 524512000
CC
    37-6 (Plastics Manufacture and Processing)
FAN.CNT 2
    PATENT NO.
                   KIND DATE APPLICATION NO. DATE
                              19830329 US 1981-266486 19810522
19810326 DE 1979-2936518 19790910
    US 4378446
                        A
     DE 2936518
                        A1
PRAI DE 1979-2936518 A
US 1980-185165 A2
                              19790910
                              19800908
CLASS
PATENT NO.
            CLASS PATENT FAMILY CLASSIFICATION CODES
US 4378446
                       C08L061-28; C08L061-32
                 INCL
                       524512000
                 IPCI
                       C08L0061-28 [ICM]; C08L0061-32 [ICS]; C08L0061-00
                       [ICS,C*]
                 TPCR
                       C08L0061-00 [I,C*]; C08L0061-00 [I,A]; B32B0027-42
                       [I,C*]; B32B0027-42 [I,A]; C08L0033-00 [I,C*];
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C08L0033-00 [I,A]; C08L0033-02 [I,A]; C08L0061-20 [I,A]; D06N0007-00 [I,C*]; D06N0007-06 [I,A]; D02H0017-00 [I,C*]; D2H0017-70 [I,C*]; D2H0017-70 [I,A]; D2H0017-43

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[I,A]; D21H0017-51 [I,A]
                 NCL.
                        524/512.000; 427/408.000; 427/415.000; 428/511.000;
                        428/514.000; 428/530.000; 524/247.000
                       D21H017/37; D21H017/43; D21H017/51
                 ECLA
 DE 2936518
                 IPCI
                       C08L0061-28 [ICM]; C08L0061-00 [ICM,C*]; C08L0033-02
                       [ICS]; C08L0033-18 [ICS]; C08L0033-00 [ICS,C*];
                       C09D0003-52 [ICS]; D06N0003-12 [ICS]; D06N0003-08
                        [ICS]; D06N0003-00 [ICS,C*]; D06N0007-06 [ICS];
                       D06N0007-00 [ICS,C*]
                 TPCR
                       C08L0061-00 [I,C*]; C08L0061-00 [I,A]; B32B0027-42
                       [I,C*]; B32B0027-42 [I,A]; C08L0033-00 [I,C*];
                       C08L0033-00 [I,A]; C08L0033-02 [I,A]; C08L0061-20
                        [I,A]; D06N0007-00 [I,C*]; D06N0007-06 [I,A];
                        D21H0017-00 [I,C*]; D21H0017-37 [I,A]; D21H0017-43
                        [I,A]; D21H0017-51 [I,A]
                       D21H017/37; D21H017/43; D21H017/51
    Low-viscosity aqueous impregnating resin solns, for use in decorative
ΔR
     laminates are prepared from 80-98% melamine resin precondensate and 2-20%
     water-soluble acrylic copolymer. Thus, 25 mL water, 39% aqueous HCHO 440,
     dimethylaminoethanol 3, 40% aqueous Na aminosulfonate 15, MeOH 35,
     iso-PrOH 25, and melamine 345 g were heated over 40 min to 90° and
     stirred 2 h at 90°. Then 54 g cocondensate of HCHO, formamide, and
     s-caprolactam was added to give a resin (I) [42231-28-7] solution
     Iso-prOH 550, water 250, CC14 8, hydroxyethyl methacrylate 182, acrylamide
     35, and acrylic acid 20 g were polymerized with 3.0 g ammonium persulfate to
     give a resin (II) [72923-48-9]. Then 1000 g I solution and 70 g II solution
     were mixed and N, N-dimethylethanolamine formate 2.8, phosphoric
     acid ester curing agent 0.56, oxyethylated nonylphenol 1.7, and water 115
     g were stirred into the resin mixture Paper was impregnated with the resin
     mixture and dried at 130-160°. The impregnated paper was pressed
     onto conventional core layers and molded 12 min at 140° at 100 bars
    to give a decorative laminate with high gloss.
ST
    melamine acrylic paper laminate
IT
    Paper
        (laminates, decorative, acrylic-melamine resin compns. for)
     42231-28-7
     RL: USES (Uses)
        (impregnating resins, containing water-soluble acrylic polymers, for
        decorative laminates)
     60451-31-2
                 72923-48-9
                             77866-27-4
                                          86435-87-2 86495-95-6
     RL: USES (Uses)
        (melamine resins containing, for decorative laminates)
             THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE
(1) Anon; US 3245932 A CAPLUS
(2) Anon; US 3976614 A CAPLUS
(3) Anon; US 3983307 A CAPLUS
(4) Anon; US 4038229 A CAPLUS
(5) Anon: US 4076896 A CAPLUS
L9
    ANSWER 35 OF 55 CAPLUS COPYRIGHT 2009 ACS on STN
AN
     1982:616701 CAPLUS
DN
    97:216701
OREF 97:36393a,36396a
ED
    Entered STN: 12 May 1984
    Polymer-supported biopolymer synthesis. 2. Phenolic
     poly(acryloylmorpholine)-based preparation of protected arginyl
     acylpeptide segments and derived arginyl peptides
AU
    Buckle, M.; Epton, R.; Marr, G.; Small, P. W.; Hudson, D.
CS
    Dep. Phys. Sci., Wolverhampton Polytech., Wolverhampton, WV1 1LY, UK
SO
    International Journal of Biological Macromolecules (1982), 4(5), 275-80
    CODEN: IJBMDR; ISSN: 0141-8130
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Journal
T.A
    English
    34-3 (Amino Acids, Peptides, and Proteins)
AB
     A new poly(acryloylmorpholine)-based phenolic support matrix, Koch-Light
     Peptide Resin A, was used for the solid (gel) phase assembly of
     polymer-bound protected arginyl acyl peptide segments. Two methods,
     selective hydrazinolysis and autocatalyzed transesterification with 2-
     dimethylaminoethanol, were used to detach the peptide segments
     from the resin. Selective hydrazinolysis illustrates the use of the
     phenolic support matrix in the preparation of arginvl acvl peptide hydrazides
     bearing hydrazine-labile nitro and benzyloxycarbonyl side chain protecting
     groups. Autocatalyzed hydrolysis in CF3CH2OH/CF3CH2ONa buffer was used to
     convert the protected arginyl acyl peptide 2-(dimethylamino)ethyl esters
     to the corresponding protected arginyl acyl peptide acids. Total
     deprotection of the latter was effected by catalytic transfer
     hydrogenation in formic acid.
ST
     arginyl peptide Merrifield synthesis; phenolic acryloylmorpholine polymer
     Merrifield support
     Merrifield synthesis
        (of arginine-containing peptides, poly(acryloylmorpholine-based phenolic
        support for)
     Peptides, preparation
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (arginine-containing, preparation of, by solid-phase method,
        poly(acryloylmorpholine-based phenolic support for)
     83713-07-9
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (as support for solid-phase synthesis of arginine peptides)
     4530-20-5DP, poly(acryoylmorpholine)-based phenolic resin-bound
     83690-45-3P
                  83690-49-7DP, poly(acryoylmorpholine)-based phenolic
     resin-bound
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (preparation and deprotection of)
     83690-56-6P
                  83690-57-7P
```

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and hydrolysis of)

83690-50-0DP, poly(acryoylmorpholine)-based phenolic resin-bound 83690-52-2DP, poly(acryovlmorpholine)-based phenolic resin-bound

83694-96-6DP, poly(acryovlmorpholine)-based phenolic resin-bound RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

(Reactant or reagent) (preparation and peptide coupling of, arginine derivative)

56-40-6DP, poly(acryoylmorpholine)-based phenolic resin-bound RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and peptide coupling of, with arginine derivative) 83690-46-4DP, poly(acryoylmorpholine)-based phenolic resin-bound

83690-47-5DP, poly(acryoylmorpholine)-based phenolic resin-bound RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

(Reactant or reagent) (preparation and peptide coupling of, with glycine derivative)

83690-51-1DP, poly(acryoylmorpholine)-based phenolic resin-bound RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and peptide coupling of, with isoleucine)

61-90-5DP, poly(acryoylmorpholine)-based phenolic resin-bound RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and peptide coupling of, with lysine derivative) 2418-80-6DP, poly(acryoylmorpholine)-based phenolic resin-bound

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79821-64-0DP, poly(acryoylmorpholine)-based phenolic resin-bound
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (preparation and peptide coupling of, with proline derivative)
     83690-45-3DP, poly(acryovlmorpholine)-based phenolic resin-bound
     83690-49-7P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (preparation and resin cleavage of)
     13139-15-6DP, poly(acryovlmorpholine)-based phenolic resin-bound
     RL: SPN (Synthetic preparation); PREP (Preparation)
       (preparation and solid-phase peptide synthesis with)
     81657-13-8P 83690-55-5P 83690-59-9P 83690-61-3P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (preparation of)
     74-79-3DP, peptides containing
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (preparation of, by solid-phase method, poly(acryloylmorpholine-based
       phenolic support for)
     4530-20-5 13139-15-6
     RL: RCT (Reactant); RACT (Reactant or reagent)
       (reaction of, with phenolic resin)
     67084-40-6 68641-29-2 83690-48-6
                                         83690-53-3 83690-54-4
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (solid-phase peptide coupling of)
    ANSWER 36 OF 55 CAPLUS COPYRIGHT 2009 ACS on STN
    1982:8219 CAPLUS
    96:8219
OREF 96:1481a,1484a
ED Entered STN: 12 May 1984
    Resin compositions for electrophoretic coating materials
PA
    Sumitomo Chemical Co., Ltd., Japan
SO
    Jpn. Kokai Tokkyo Koho, 12 pp.
    CODEN: JKXXAF
DT
    Patent
    Japanese
    ICM C09D005-25
    ICS C09D003-72
    42-7 (Coatings, Inks, and Related Products)
FAN.CNT 1
                     KIND DATE
                                        APPLICATION NO. DATE
    PATENT NO.
                      ----
                             _____
                                        -----
PI JP 56106973 A
JP 61057352 B
PRAI JP 1980-9202 A
                             19810825 JP 1980-9202
                             19861206
                              19800128
CLASS
PATENT NO. CLASS PATENT FAMILY CLASSIFICATION CODES
 _____
               ICM C09D005-25
JP 56106973
                ICS
                     C09D003-72
                IPCI C09D0005-25; C09D0003-72
    Coating materials for cathode electrodeposition are prepared from the
     reaction products of a modified polybutadiene with phenol, epoxy resins,
     and partially blocked organic polyisocyanates. Thus, maleated liquid
     polybutadiene 100, phenol 50, toluene 30.1, and BF3. phenol 0.36 g were
     heated 140 min at 80-90° to phenol conversion 20.5%, treated with
     Et3N to deactivate the catalyst, diluted with 33.9 g ethylene glycol mono-Et
     acetate (I), mixed (92.4 g) with bisphenol A-epichlorohydrin copolymer
```

(II) 130, Et2NH 6.4, and I 58.2 g, heated 3 h at 120°, mixed with 21.9 g acrylic acid and 1 g hydroquinone, heated 5 h at 100°, mixed with 113.9 g solution of N,N-dimethylaminoethanol-half-blocked TDI in I, stirred 2 h at 70°, mixed with 10 g Et Cellosolve, heated 1 h

ΤТ

1.9

AN

DN

ΤI

LA

IC

AB

at 70°, mixed (380 parts) with 167 parts master batch containing the reaction product of II acrylate with the half-blocked TDI 12 parts, 85% formic acid, and H2O, and used to form a coating on steel (carbon anode) having good appearance, pencil hardness 2H, Erichsen test >8 mm, du Pont impact resistance (0.5 in., 0.5 kg) >50, and good resistance to iso-BuCOMe, water, and corrosion.

- ST cathode electrodeposition coating material; maleated polybutadiene coating material; epoxy acrylate coating material; ethylaminoethanol blocked TDI coating
- IT Coating materials

(electrophoretic, containing acrylic acid-bisphenol A-epichlorohydrin copolymer-diethylaminoethanol-half-blocked TDI-maleated polybutadiene-phenol reaction products)

T 79-10-7D, reaction products with bisphenol A-epichlorohydrin copolymer, diethylaminoethanol-half-blocked TDI, maleated polybutadiene, and phenol 108-95-2D, reaction products with acrylic acid, bisphenol A-epichlorohydrin copolymer, diethylaminoethanol-half-blocked TDI, and maleated polybutadiene 9003-17-2D, maleated, reaction products with acrylic acid, bisphenol A-epichlorohydrin copolymer, diethylaminoethanol-half-blocked TDI, and phenol 25068-38-6D, reaction products with acrylic acid, diethylaminoethanol-half-blocked TDI, maleated polybutadiene, and phenol 67391-91-7D, reaction products with acrylic acid, bisphenol A-epichlorohydrin copolymer, maleated polybutadiene, and phenol

RL: TEM (Technical or engineered material use); USES (Uses) (coatings, electrophoretic)

- L9 ANSWER 37 OF 55 CAPLUS COPYRIGHT 2009 ACS on STN
- AN 1981:534178 CAPLUS
- DN 95:134178
- OREF 95:22471a,22474a
- ED Entered STN: 12 May 1984
- TI Modified isocyanate compositions
- IN Hughes, Jeffrey; Murray, Gerard John PA Imperial Chemical Industries Ltd., UK
- SO Eur. Pat. Appl., 21 pp.
 - CODEN: EPXXDW

PATENT NO.

- DT Patent
- LA English
- IC C08G018-77; C07C123-00
- CC 38-2 (Elastomers, Including Natural Rubber)

KIND DATE

FAN.CNT 1

PI	EP	32011		A1	19810715	EP	1980-304506	19801212		
	EΡ	32011		B1	19840822					
		R: BE,	DE, FR,	GB, IT,	, NL					
	GB	2068368		A	19810812	GB	1980-39820	19801212		
	GB	2068368		В	19840404					
	JP	56100753		A	19810812	JP	1980-184177	19801226		
	US	4322364		A	19820330	US	1981-222143	19810102		
PRAI	GB	1980-12		A	19800102					
CLASS	3									
PATE	ENT	NO.	CLASS	PATENT I	FAMILY CLASS:	IFIC	CATION CODES			
EP 3	3201	.1	IC	C08G018-77; C07C123-00						
			IPCI	C08G0018	B-77 [ICM]; (C080	G0018-00 [ICM,C*]; C	07C0123-00		
				[ICS]						
			IPCR	C07D0229	9-00 [I,C*];	C07	D0229-00 [I,A]; C070	C0067-00		
				[I,C*];	C07C0067-00	[I,	A]; C07C0241-00 [I,0	C*];		
				C07C024	1-00 [I,A]; (2070	C0267-00 [I,C*]; C070	C0267-00		
				[I,A]; (C08G0018-00	[I,0	C*]; C08G0018-78 [I,	A];		

APPLICATION NO.

DATE

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C08G0018-79 [I,A]
                ECLA
                       C08G018/78; C08G018/79G
GB 2068368
                IPCI
                       C07C0123-00 [ICM]; C08G0018-78 [ICS]; C08G0018-00
                       [ICS,C*]
                IPCR
                       C07D0229-00 [I,C*]; C07D0229-00 [I,A]; C07C0067-00
                       [I,C*]; C07C0067-00 [I,A]; C07C0241-00 [I,C*];
                       C07C0241-00 [I,A]; C07C0267-00 [I,C*]; C07C0267-00
                       [I,A]; C08G0018-00 [I,C*]; C08G0018-78 [I,A];
                       C08G0018-79 [I,A]
                       C07C0119-055 | ICM|; C07D0229-00 | ICS|; C08G0018-78
JP 56100753
                IPCI
                       | ICA|; C08G0018-00 | ICA, C*|
                IPCR
                       C07D0229-00 [I,C*]; C07D0229-00 [I,A]; C07C0067-00
                       [I,C*]; C07C0067-00 [I,A]; C07C0241-00 [I,C*];
                       C07C0241-00 [I,A]; C07C0267-00 [I,C*]; C07C0267-00
                       [I,A]; C08G0018-00 [I,C*]; C08G0018-78 [I,A];
                       C08G0018-79 [I.A]
US 4322364
                TPCT
                       C07C0119-048 | ICM|; C07C0119-055 | ICS|
                IPCR
                       C07C0265-00 [I,C*]; C07C0265-12 [I,A]; C08G0018-00
                       [I,C*]; C08G0018-78 [I,A]
                NCL
                       560/351.000; 521/162.000; 528/044.000; 548/951.000;
                       560/035.000; 560/168.000
                ECLA
                       C07C118/00A4; C08G018/78
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Modified isocvanates are manufactured by treating compns. containing carbodiimide

groups and free NCO groups with a diester of an aliphatic dicarboxylic acid in the presence of oxalic acid [110-40-7] or HCHO [64-18-6]. Liquid diphenylmethane diisocyanate compns. prepared by the process are storage stable and do not form a sediment on standing. The increase of NCO functionality and viscosity associated with the formation of uretonimine groups is minimized. Thus, 250 parts 4,4'-diphenylmethane diisocyanate was heated to 50° under N, 0.1 part dimethylaminoethanol was added, and the mixture was heated to 105° in 15 min. After adding 0.00125 part 1-phenyl-3-Me phospholene, the mixture was stirred at 105° until the NCO value was 30° and then treated with 16 parts 5:1 di-Et oxalate-oxalic acid mixture and 0.0375 part SOC12 to give a pale yellow liquid having viscosity 70 cp at 25° and final NCO value 26.5%. The product remained liquid even on prolonged storage at 0° and IR anal. showed there was no absorption at 1360 cm-1 (indicating the absence of uretonimine groups.). A microcellular elastomer prepared from the modified isocvanate and polvethylene-polypropylene glycol, polyethylene-polypropylene glycol ether with glycerol, 1,4-butanediol, and ethylene glycol had d. 540 kg/m2. Shore A hardness 71, tensile strength 3220 kN/m2, and elongation at break 230%.

urethane rubber foam; cellular polyurethane modified diisocyanate; ST diphenylmethane diisocyanate carbodiimide modified; oxalate diisocyanate modification; formic acid dissocvanate modification

Rubber, urethane, preparation

Urethane polymers, preparation

RL: PREP (Preparation)

(cellular, aliphatic dicarboxylic acid diester-modified diphenylmethane diisocyanates for manufacture of, storage-stable)

- 64-18-6, uses and miscellaneous 110-40-7D, reaction products with diphenylmethane diisocvanate, polymers with glycols, polyoxyalkylenes and polyoxyalkylene ethers RL: USES (Uses)
 - (diisocyanate modification with aliphatic dicarboxylic acid diesters in presence of)
- 95-92-1D, reaction products with diphenylmethane diisocyanate, polymers with glycols, polyoxyalkylenes and polyoxyalkylene ethers 101-68-8D, reaction products with aliphatic dicarboxylic acid diesters, polymers with glycols, polyoxyalkylenes and polyoxyalkylene ethers 105-53-3D, reaction products with diphenylmethane diisocyanate, polymers with glycols,

polyoxyalkylenes and polyoxyalkylene ethers 106-65-0D, reaction products with diphenylmethane diisocyanate, polymers with glycols, polyoxyalkylenes and polyoxyalkylene ethers 107-21-1D, polymers with aliphatic dicarboxylic acid diester-modified diphenylmethane diisocyanates 110-63-4D, polymers with aliphatic dicarboxylic acid diester-modified diphenylmethane diisocyanates 2536-05-2D, reaction products with aliphatic dicarboxylic acid diesters, polymers with glycols, polyoxyalkylenes and polyoxyalkylene ethers 3155-16-6D, reaction products with diphenylmethane diisocyanate, polymers with glycols, polyoxyalkylenes and polyoxyalkylene ethers 5873-54-1D, reaction products with aliphatic dicarboxylic acid diesters, polymers with glycols, polyoxyalkylenes and polyoxyalkylene ethers 9003-11-6D, polymers with aliphatic dicarboxylic acid diester-modified diphenylmethane diisocyanates 9082-00-2D, polymers with aliphatic dicarboxylic acid diester-modified diphenylmethane diisocyanates 15779-81-4D, reaction products with diphenylmethane diisocyanate, polymers with glycols, polyoxyalkylenes and polyoxyalkylene ethers 67385-13-1D, reaction products with diphenylmethane diisocyanate, polymers with glycols, polyoxyalkylenes and polyoxyalkylene ethers RL: USES (Uses) (rubber)

(100061

- L9 ANSWER 38 OF 55 CAPLUS COPYRIGHT 2009 ACS on STN
- AN 1981:210587 CAPLUS
- DN 94:210587
- OREF 94:34452h,34453a
- ED Entered STN: 12 May 1984
- TI Storage-stable acrylate-modified melamine resin and its use
- IN Adam, Wilhelm; Wagner, Curt A.; Konrad, Renate; Engelhardt, Friedrich; Riegel, Ulrich; Eckardt, Georg Wolfgang; Piesch, Steffen

PATENT NO. KIND DATE APPLICATION NO. DATE

- PA Cassella A.-G., Fed. Rep. Ger.
- SO Ger. Offen., 29 pp.
- CODEN: GWXXBX DT Patent
- LA German
- IC C08L061-28; C08L033-02; C08L033-18; C09D003-52
- CC 43-7 (Cellulose, Lignin, Paper, and Other Wood Products) FAN.CNT 2

790910
800830
800830
800909
810522
810522
2
0033-02
1;
3-08
3-08 1;
3-08
3-08 1;

[I,A]; D06N0007-00 [I,C*]; D06N0007-06 [I,A];

```
D21H0017-00 [I,C*]; D21H0017-37 [I,A]; D21H0017-43
                       [I,A]; D21H0017-51 [I,A]
                ECLA
                       D21H017/37; D21H017/43; D21H017/51
EP 26841
                IPCI
                       C08L0061-32 [ICM]; D21H0003-56 [ICA]; C08L0061-32
                       [ICI]; C08L0061-00 [ICI,C*]; C08L0033-04 [ICI];
                       C08L0033-00 [ICI,C*]
                IPCR
                       C08L0061-00 [I,C*]; C08L0061-00 [I,A]; B32B0027-42
                       [I,C*]; B32B0027-42 [I,A]; C08L0033-00 [I,C*];
                       C08L0033-00 [I,A]; C08L0033-02 [I,A]; C08L0061-20
                       [I,A]; D06N0007-00 [I,C*]; D06N0007-06 [I,A];
                       D21H0017-00 [I,C*]; D21H0017-37 [I,A]; D21H0017-43
                       [I,A]; D21H0017-51 [I,A]
                ECLA
                       D21H017/37; D21H017/43; D21H017/51
AT 7507
                IPCI
                       C08L0061-32 [ICM]; C08L0061-00 [ICM,C*]
                IPCR
                       C08L0061-00 [I,C*]; C08L0061-32 [I,A]
JP 56045943
                IPCI
                       C08L0061-28 [ICM]; C08L0061-00 [ICM,C*]; B32B0027-42
                       [ICS]
                IPCR
                       C08L0061-00 [I,C*]; C08L0061-00 [I,A]; B32B0027-42
                       [I,C*]; B32B0027-42 [I,A]; C08L0033-00 [I,C*];
                       C08L0033-00 [I,A]; C08L0033-02 [I,A]; C08L0061-20
                       [I,A]; D06N0007-00 [I,C*]; D06N0007-06 [I,A];
                       D21H0017-00 [I,C*]; D21H0017-37 [I,A]; D21H0017-43
                       [I,A]; D21H0017-51 [I,A]
US 4378446
                IPCI
                       C08L0061-28 | ICM|; C08L0061-32 | ICS|; C08L0061-00
                       LICS,C*1
                       C08L0061-00 [I,C*]; C08L0061-00 [I,A]; B32B0027-42
                TPCR
                       [I,C*]; B32B0027-42 [I,A]; C08L0033-00 [I,C*];
                       C08L0033-00 [I,A]; C08L0033-02 [I,A]; C08L0061-20
                       [I,A]; D06N0007-00 [I,C*]; D06N0007-06 [I,A];
                       D21H0017-00 [I,C*]; D21H0017-37 [I,A]; D21H0017-43
                       [I.A]; D21H0017-51 [I.A]
                NCL
                       524/512.000; 427/408.000; 427/415.000; 428/511.000;
                       428/514.000; 428/530.000; 524/247.000
                ECLA
                       D21H017/37; D21H017/43; D21H017/51
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 $\ensuremath{\mathsf{AB}}$. Storage-stable, low-viscosity aqueous impregnating resin solns. for the manufacture

of laminates and wood products with improved weather resistance contain melamine resins and water-soluble acrylate polymers. Thus, 440 g 39% HCHO, 25 mL water, 3 g dimethylaminoethanol (1) [108-01-0], 15 g 40% Na amidosulfonic acid, 35 MeOH, 25 g iso-PrOH, and 345 g melamine were heated 2 h at 90° to give a clear resin [25036-13-9] solution, having water dilution capacity 1:20, which was mixed with 54 g water and 54 g 1:9:5 s-caprolactam-formamide-formaldehyde copolymer [71092-18-7] of give resin solution A. A solution of 3.0 g (NH4)25208 in 50 g water was added in 5-mL portions to a clear monomer solution containing iso-PrOH 550, water

250,

CC14 8, hydroxyethyl methacrylate 182, acrylamide 35, and acrylic acid 20 g and the composition was polymerized under N, mixed with 20 g I, and distilled to

give a viscous polymer solution which was diluted with 200 mL water and 10 g I to produce solution B having pH 6.5-7 and solids content 40%. A mixture containing

1000 g A and 70 g B was combined with N,N-dimethylethanolamine formate 2.8, polyphosphoric acid ester hardener 0.56, polyethylene glycol alkylphenyl ether assistant 1.7, and water 115 g to give .apprx.1190 g impregnating solution (C) with solids content .apprx.50% and viscosity 15-20 s (DIN 53 211) at 20°. Paper (80 g/m2) impregnated with C and dried to give a resin content of 60% and moisture content of 5-6% was pressed for 12 min at 140° and 100 bar with a phenolic resin laminate. The decorative product lost 50% of its gloss after 3500 h exposure to UV light.

ST melamine resin impregnation paper; acrylate polymer impregnation paper;

paper protective layer laminate; wood laminate protective layer; phenolic resin laminate; laminate weather resistant

IT Wood

(decorative laminates from, resin-impregnated paper as protective layers for weather-resistant meltamine resin-acrylate polymer impregnating compns. for)

IT Paper

(impregnation of, melamine resin-acrylate polymer compns. for, in weather-resistant decorative laminate and wood product manufacture)

IT Phenolic resins, uses and miscellaneous

RL: USES (Uses)

(laminates, resin-impregnated paper as protective layers for weather-resistant, melamine resin-acrylate polymer impregnating compns. for)

IT 71092-18-7

RL: USES (Uses)

(impregnating solns. containing, for paper in weather-resistant decorative laminate and wood product manufacture)

IT 25036-13-9 77817-95-9

RL: USES (Uses)

(impregnating solns., containing acrylate copolymers, for paper in weather-resistant decorative laminate and wood product manufacture)

IT 72923-48-9 77866-27-4

RL: USES (Uses)

(impregnating solns., containing melamine resins, for paper in weather-resistant decorative laminate and wood product manufacture)

IT 108-01-0 RL: USES (Uses)

(in manufacture of storage-stable acrylate-modified melamine resins)

L9 ANSWER 39 OF 55 CAPLUS COPYRIGHT 2009 ACS on STN

AN 1980:604705 CAPLUS

DN 93:204705

OREF 93:32669a,32672a

ED Entered STN: 12 May 1984

TI 4,1-Benzoxazepine or 4,1-benzothiazepine derivatives

IN Hirai, Kentaro; Matsutani, Shigeru; Ishiba, Teruyuki; Makino, Itsuo

PA Shionogi and Co., Ltd., Japan

SO Ger. Offen., 57 pp.

CODEN: GWXXBX

DT Patent LA German

IC C07D498-04; C07D513-04; C07D267-14; A61K031-55

CC 28-24 (Heterocyclic Compounds (More Than One Hetero Atom))

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	DE 2947773	A1	19800604	DE 1979-2947773	19791127
	JP 55072177	A	19800530	JP 1978-146949	19781127
	JP 62031719	В	19870709		
	CA 1127639	A1	19820713	CA 1979-339060	19791102
	US 4297280	A	19811027	US 1979-91814	19791106
	ZA 7906040	A	19801029	ZA 1979-6040	19791109
	AU 7952993	A	19800529	AU 1979-52993	19791120
	AU 533517	B2	19831201		
	CH 642647	A5	19840430	CH 1979-10423	19791122
	DK 7905001	A	19800528	DK 1979-5001	19791123
	SE 7909751	A	19800528	SE 1979-9751	19791126
	FR 2442239	A1	19800620	FR 1979-29096	19791126
	FR 2442239	B1	19830701		
	HU 21864	A2	19820227	HU 1979-SI1731	19791126
	HU 179589	В	19821129		
	FR 2442239 FR 2442239 HU 21864	A1 B1 A2	19800620 19830701 19820227	FR 1979-29096	197911

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PATENT NO.	CLASS		ASSIFICATION CODES	
DE 2947773	IC IPCI	0070498-04; 0071 070498-04 [ICI [ICS]; 00700513- 0700267-001 [ICI [ICS]; 00700513- 0700267-001 [ICI [IC,4]; A6180033- 08180031-095 [ICI [IC,4]; A6180033- 08190025-08 [IC,4]; A6190025- 08100249-10 [IC,4]; A6190025- 0700249-10 [IC,4]; A6190025- 0700249-10 [IC,4]; C0700249- 0700281-001 [IC,4]; C0700281- 01[IC,4]; C0700281- 01[IC,4]; C0700281- 01[IC,6]; C0700521-	.513-04; C07D267-14; A6: 41; C07D0498-00 [ICM, C*; -00 [ICS, C*]; C07D0267-1 5, C*1; A61K0031-55 [ICS, -C*1; A61K0031-55 [ICS, -C*1; A61K0031-55 [IC, A] -4196 [I, A]; A61K0031-55 -554 [I, C*1; A61K0031-55 -554 [I, C*1; A61K0031-55 -554 [I, C*1; A61K0031-55 -50 [I, A]; A61P0025-02 -00 [I, A]; A61P0025-02 -00 [I, A]; C07D0249-08 -00 [I, C*1; C07D0249-08 -00 [I, C*1; C07D0237-00 -2*1; C07D0281-10 [I, A]; -36 [I, A]; C07D0498-00 -01; C07D0513-00 [I, C*1]; -00 [I, C*1; C07D0521-00	IRO31-55 ; CO7D0513-04 44 [ICS]; , A61K0031-4196 55 [I,C*]; ; A61K0031-553 54 [I,A]; A61F0025-00 [I,A]; G1F0025-22 [I,A]; C07D0267-14 [I,A]; C07D0285-00 [I,C*]; C07D0513-04 [I,C*];
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	NCL ECLA	540/548.000; 540/490.000; 540/552.000 COTD249/08C2D; COTD249/10; COTD267/14; COTD273/00J; COTD285/36; COTD498/04+267C-235C; COTD498/04+267C+249C; COTD498/04+267C+253C; COTD513/04+281C+249C;
ZA 7906040	IPCI IPCR	C07D513/04+281C+255C; C07D521/00B2E C07D I[CM]; A6IK [ICS] A6IK0031-395 [I,C*]; A6IK0031-395 [I,A]; A6IK0031-4196 I[,C*]; A6IK0031-4196 [I,A]; A6IK0031-55 [I,C*]; A6IK0031-55 [I,A]; A6IK0031-553 [I,C*]; A6IK0031-553 I[,A]; A6IK0031-554 [I,A]; A6IK0031-554 [I,A]; A6IP0021-00 [I,C*]; A6IP0021-02 [I,A]; A6IP0025-02 I[,C*]; A6IP0025-00 [I,A]; A6IP0025-02 [I,A]; A6IP0025-08 [I,A]; A6IP0025-20 [I,A]; A6IP0025-22 I[,A]; C07D0249-01 [I,C*]; C07D0249-08 [I,A]; C07D0249-10 [I,A]; C07D0267-00 [I,C*]; C07D0267-14 I[,A]; C07D0233-30 [I,C*]; C07D0273-00 [I,A]; C07D0289-04 [I,A]; C07D0281-00 [I,C*]; C07D0385-30 I[,C*]; C07D0385-36 [I,A]; C07D048-00 [I,C*]; C07D049-04 [I,A]; C07D0513-00 [I,C*]; C07D0513-04 I[,A]; C07D0285-36 [I,A]; C07D0567-10 [I,A]; C07D0496-20 [I,C*]; C07D0571-00 [I,A]; C07D0496-36 [I,A]; C07D0513-00 [I,A]; C07D285/36; C07D498/04+267C+235C; C07D498/04+267C+249C; C07D498/04+267C+235C; C07D513/04+28IC-249C;
AU 7952993	IPCI	C07D513/04+281C+253C; C07D521/00B2E C07D0267-14 [ICM]; C07D0267-00 [ICM,C*]; C07D0281-10 [ICS]; C07D0281-00 [ICS,C*]; C07D0498-04 [ICS]; C07D0498-00 [ICS,C*]; C07D0513-04 [ICS]; C07D0513-00
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FR 2442239	IPCI	C07D513/04+281C+253C; C07D521/00B2E C07D0498-04 [ICM]; C07D0498-00 [ICM,C*]; C07D0267-14 [ICS]; C07D0267-00 [ICS,C*]; C07D0513-04 [ICS]; C07D0513-00 [ICS,C*]; A6IK0031-55 [ICS]
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		[I,A]; C07D0273-00 [I,C*]; C07D0273-00 [I,A];
		C07D0281-00 [I,C*]; C07D0281-10 [I,A]; C07D0285-00
		[I,C*]; C07D0285-36 [I,A]; C07D0498-00 [I,C*];
		C07D0498-04 [I,A]; C07D0513-00 [I,C*]; C07D0513-04 [I,A]; C07D0521-00 [I,C*]; C07D0521-00 [I,A]
DD 147360	IPCI	C07D0498-04 [ICM]; C07D0498-00 [ICM,C*]; C07D0513-04
		[ICA]; C07D0513-00 [ICA,C*]; C07D0267-14 [ICA];
		C07D0267-00 [ICA,C*]; C07D0281-10 [ICA]; C07D0281-00
	IPCR	[ICA,C*] A61K0031-395 [I,C*]; A61K0031-395 [I,A]; A61K0031-4196
		[I,C*]; A61K0031-4196 [I,A]; A61K0031-55 [I,C*];
		A61K0031-55 [I,A]; A61K0031-553 [I,C*]; A61K0031-553
		[I,A]; A61K0031-554 [I,C*]; A61K0031-554 [I,A]; A61P0021-00 [I,C*]; A61P0021-02 [I,A]; A61P0025-00
		[I,C*]; A61P0025-00 [I,A]; A61P0025-02 [I,A];
		A61P0025-08 [I,A]; A61P0025-20 [I,A]; A61P0025-22
		[I,A]; C07D0249-00 [I,C*]; C07D0249-08 [I,A];
		C07D0249-10 [I,A]; C07D0267-00 [I,C*]; C07D0267-14
		[I,A]; C07D0273-00 [I,C*]; C07D0273-00 [I,A]; C07D0281-00 [I,C*]; C07D0281-10 [I,A]; C07D0285-00
		[I,C*]; C07D0285-36 [I,A]; C07D0498-00 [I,C*];
		C07D0498-04 [I,A]; C07D0513-00 [I,C*]; C07D0513-04
	DOT 1	[I,A]; C07D0521-00 [I,C*]; C07D0521-00 [I,A]
	ECLA	C07D249/08C2D; C07D249/10; C07D267/14; C07D273/00J; C07D285/36; C07D498/04+267C+235C; C07D498/04+267C+249C;
		C07D498/04+267C+253C; C07D513/04+281C+249C;
		C07D513/04+281C+253C; C07D521/00B2E
SU 936815	IPCI	C07D0498-04 [ICM]; C07D0498-00 [ICM,C*]; C07D0513-04
		[ICS]; C07D0513-00 [ICS,C*]; A61K0031-41 [ICS]; A61K0031-53 [ICS]; A61K0031-55 [ICS]
	IPCR	A61K0031-395 [I,C*]; A61K0031-395 [I,A]; A61K0031-4196
		[I,C*]; A61K0031-4196 [I,A]; A61K0031-55 [I,C*];
		A61K0031-55 [I,A]; A61K0031-553 [I,C*]; A61K0031-553
		[I,A]; A61K0031-554 [I,C*]; A61K0031-554 [I,A]; A61P0021-00 [I,C*]; A61P0021-02 [I,A]; A61P0025-00
		[I,C*]; A61P0025-00 [I,A]; A61P0025-02 [I,A];
		A61P0025-08 [I,A]; A61P0025-20 [I,A]; A61P0025-22
		[I,A]; C07D0249-00 [I,C*]; C07D0249-08 [I,A];
		C07D0249-10 [I,A]; C07D0267-00 [I,C*]; C07D0267-14 [I,A]; C07D0273-00 [I,C*]; C07D0273-00 [I,A];
		C07D0281-00 [I,C*]; C07D0281-10 [I,A]; C07D0285-00
		[I,C*]; C07D0285-36 [I,A]; C07D0498-00 [I,C*];
		C07D0498-04 [I,A]; C07D0513-00 [I,C*]; C07D0513-04
		[I,A]; C07D0521-00 [I,C*]; C07D0521-00 [I,A]

SU 1005660 TPCT C07D0267-14 [ICM]; C07D0267-00 [ICM,C*]; C07D0281-10 [ICS]; C07D0281-00 [ICS,C*]; C07D0498-04 [ICS]; C07D0498-00 [ICS,C*]; C07D0513-04 [ICS]; C07D0513-00 [ICS,C*]; A61K0031-41 [ICS]; A61K0031-53 [ICS];

A61K0031-55 [ICS]

IPCR A61K0031-395 [I,C*]; A61K0031-395 [I,A]; A61K0031-4196 [I,C*]; A61K0031-4196 [I,A]; A61K0031-55 [I,C*]; A61K0031-55 [I,A]; A61K0031-553 [I,C*]; A61K0031-553 [I,A]; A61K0031-554 [I,C*]; A61K0031-554 [I,A]; A61P0021-00 [I,C*]; A61P0021-02 [I,A]; A61P0025-00 |I,C*|; A61P0025-00 |I,A|; A61P0025-02 |I,A|; A61P0025-08 [I,A]; A61P0025-20 [I,A]; A61P0025-22 [I,A]; C07D0249-00 [I,C*]; C07D0249-08 [I,A]; C07D0249-10 [I,A]; C07D0267-00 [I,C*]; C07D0267-14 [I,A]; C07D0273-00 [I,C*]; C07D0273-00 [I,A]; C07D0281-00 [I,C*]; C07D0281-10 [I,A]; C07D0285-00 [I,C*]; C07D0285-36 [I,A]; C07D0498-00 [I,C*]; C07D0498-04 [I,A]; C07D0513-00 [I,C*]; C07D0513-04 [I,A]; C07D0521-00 [I,C*]; C07D0521-00 [I,A]

US 4341704 IPCI C07D0513-04 [ICM]; C07D0513-00 [ICM,C*] IPCR

A61K0031-395 [I,C*]; A61K0031-395 [I,A]; A61K0031-4196 [I,C*]; A61K0031-4196 [I,A]; A61K0031-55 [I,C*]; A61K0031-55 [I,A]; A61K0031-553 [I,C*]; A61K0031-553 [I,A]; A61K0031-554 [I,C*]; A61K0031-554 [I,A]; A61P0021-00 [I,C*]; A61P0021-02 [I,A]; A61P0025-00 [I,C*]; A61P0025-00 [I,A]; A61P0025-02 [I,A]; A61P0025-08 [I,A]; A61P0025-20 [I,A]; A61P0025-22 [I,A]; C07D0249-00 [I,C*]; C07D0249-08 [I,A]; C07D0249-10 [I,A]; C07D0267-00 [I,C*]; C07D0267-14 [I,A]; C07D0273-00 [I,C*]; C07D0273-00 [I,A]; C07D0281-00 [I,C*]; C07D0281-10 [I,A]; C07D0285-00 [I,C*]; C07D0285-36 [I,A]; C07D0498-00 [I,C*];

C07D0498-04 [I,A]; C07D0513-00 [I,C*]; C07D0513-04 [I,A]; C07D0521-00 [I,C*]; C07D0521-00 [I,A] 540/548.000; 540/490.000; 540/552.000 NCL ECLA C07D249/08C2D; C07D249/10; C07D267/14; C07D273/00J;

C07D285/36; C07D498/04+267C+235C; C07D498/04+267C+249C; C07D498/04+267C+253C; C07D513/04+281C+249C; C07D513/04+281C+253C; C07D521/00B2E

CASREACT 93:204705; MARPAT 93:204705

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Ι

AB The title compds. I [X = O, S; RX1 = CR4:NN:, N:CR5N:, COC(:CHR6)N:,COCR7:NN:; X1 = O, S; R = H, alkyl, aralkyl; R1 = H, halogen; R2 = halogen, NO2; R3 = H, alkoxy, dialkylaminoalkoxy; R4 = alkyl, aminoalkyl; R5 = dialkylaminoacyl; R6 = dialkylamino, 4-alkylpiperazino; R7 = alkyl]

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were prepared Thus, 5,2-C1(H2N)C6H3COC6H4C1-2 was acylated with C1CH2COC1,
5,2-C1(C1CH2CONH)C6H3COC6H4C1-2 reduced to the alc., and cyclized with
Me2CHONa to give I (X = X1 = O, R = R3 = H, R1 = R2 = C1). The latter
compound was converted to the thione and treated with AcNHNH2 to give I (X =
O, X1 = NNHAc, R = R3 = H, R1 = R2 = C1), which was cyclized with acid to
I (X = 0, RX1 = CMe:NN:, R1 = R2 = C1, R3 = H; II). II had ED50 of 0.74
and 30.6 mg/kg resp. in the pentetrazole and rotating rod tests.
benzoxazepine; benzothiazepine; sedative benzothiazepine benzoxazepine;
muscle relaxant benzoxazepine benzothiazepine; triazolobenzoxazepine;
imidazobenzoxazepine; triazinobenzoxazepine
Hypnotics and Sedatives
Muscle relaxants and Spasmolytics
   (benzoxazepine and benzothiazepine derivs.)
2958-36-3
RL: RCT (Reactant); RACT (Reactant or reagent)
   (acvlation of)
79-04-9
RL: RCT (Reactant); RACT (Reactant or reagent)
   (acylation of aminobenzophenone derivative by)
54196-62-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
   (preparation and chlorination of)
75450-23-6P
              75450-26-9P 75450-37-2P
                                         75450-42-9P 75450-50-9P
75459-11-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
   (preparation and cyclization of)
57998-42-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
   (preparation and cyclization of, with potassium ethoxide)
62293-36-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
   (preparation and cyclization of, with potassium methoxide)
75450-46-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
   (preparation and cyclization of, with sodium ethoxide)
75450-31-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
   (preparation and deblocking of)
54196-61-1P
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ST

ΤТ

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and methylolation of)

75450-32-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and oxidation of)

75450-40-7P 75450-43-0P

> RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(preparation and pharmacol. activity of)

75450-38-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation and reaction of, with DMF di-Me acetal)

75450-25-8P 75450-35-0P

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RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
   (preparation and reaction of, with acetylhydrazine)
75450-28-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
   (preparation and reaction of, with azide)
74067-45-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
   (preparation and reaction of, with carbon disulfide)
75450-33-8P 75450-45-2P
                           75450-49-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
   (preparation and reaction of, with chloroacetyl chloride)
75450-41-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
   (preparation and reaction of, with pyruvic acid)
14405-03-9P 75450-29-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
   (preparation and reduction of)
75450-62-3P 75459-13-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
   (preparation and sedative and muscle relaxant activity of)
75450-24-7P 75450-34-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
   (preparation and thiolation of)
75450-30-5P
             75450-36-1P 75450-44-1P
                                          75450-47-4P
                                                        75450-48-5P
75450-51-0P
             75450-52-1P
                           75450-53-2P
                                          75450-54-3P
                                                        75450-55-4P
75450-56-5P
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                                          75450-59-8P
                                                        75450-60-1P
             75459-12-0P
75450-61-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
   (preparation of)
75450-27-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
   (preparation, bromination, and pharmacol, activity of)
RL: SPN (Synthetic preparation); PREP (Preparation)
   (preparation, reaction with methylpiperazine, and pharmacol. activity of)
75-15-0, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
   (reaction of, with aminophenyl carbinol)
64-18-6, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
   (reaction of, with aminoquinazoline)
56-40-6, reactions 302-01-2, reactions
                                           1068-57-1
RL: RCT (Reactant); RACT (Reactant or reagent)
   (reaction of, with benzoxazepinethione)
5680-83-1
RL: RCT (Reactant); RACT (Reactant or reagent)
   (reaction of, with benzoxazepinethione derivative)
127-17-3, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
   (reaction of, with benzoxazepinone hydrazone)
54567-12-3 65698-99-9
RL: RCT (Reactant); RACT (Reactant or reagent)
   (reaction of, with chloroacetyl chloride)
108-01-0
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RL: RCT (Reactant); RACT (Reactant or reagent)
         (reaction of, with chloroacetylaminobenzophenone derivative)
      63480-61-5
      RL: RCT (Reactant); RACT (Reactant or reagent)
         (reaction of, with dimethylaminoethanol)
      109-01-3
      RL: RCT (Reactant); RACT (Reactant or reagent)
         (reaction of, with dimethylaminomethyleneimidazobenzoxazepinone)
      54567-12-3
      RL: RCT (Reactant); RACT (Reactant or reagent)
         (reaction of, with formic acid)
      4637-24-5
      RL: RCT (Reactant); RACT (Reactant or reagent)
         (reaction of, with imidazobenzoxazepinone)
 1.9
      ANSWER 40 OF 55 CAPLUS COPYRIGHT 2009 ACS on STN
 ΔN
     1976:525819 CAPLUS
 DN 85:125819
 OREF 85:20189a,20192a
     Entered STN: 12 May 1984
      Leather tanning using hydrophilic oligourethanes
 IN
    Traeubel, Harro; Reiff, Helmut; Dieterich, Dieter
    Bayer A.-G., Fed. Rep. Ger.
 PA
 SO
    Ger. Offen., 22 pp.
     CODEN: GWXXBX
     Patent
 T.A
     German
     C14C003-18
 IC
41-3 (Leather and Related Materials)
                                                                 DATE
                                           APPLICATION NO.
                                           -----
                                                                 19750131
                                                                  19750327
                                                                19750402
                                                                  19750402
                                                                  19750403
  DE 2504081
                IC C14C003-18
                 IPCI C14C0003-18 [ICM]; C14C0003-00 [ICM,C*]
                  IPCR C08G0018-00 [I,C*]; C08G0018-08 [I,A]; C14C0003-00
                        [I,C*]; C14C0003-18 [I,A]; D06P0001-44 [I,C*];
                         D06P0001-52 [I,A]; D06P0001-64 [I,C*]; D06P0001-649
                        [I,A]
                 ECLA C08G018/08B; C14C003/18; D06P001/52D6; D06P001/649D
  FR 2266743
                 IPCI C14C0003-18 [ICM]; C14C0003-00 [ICM,C*]
IPCI C14C0003-18 [ICM]; C14C0003-00 [ICM,C*]
  DD 117477
                  IPCR C14C0003-00 [I,C*]; C14C0003-18 [I,A]
                 ECLA C14C003/18
  GB 1495598
                 IPCI C14C0003-18 [ICM]; C14C0003-16 [ICS]; C14C0003-00
                [ICS,C*]; C08G0018-06 [ICS]; C08G0018-00 [ICS,C*]

IPCR C14C0003-00 [I,C*]; C14C0003-18 [I,A]
  BR 7502008
                IPCI C14C0003-18 [ICM]; C14C0003-00 [ICM,C*]
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TPCP
                       C14C0003-00 [I,C*]; C14C0003-18 [I,A]
US 4106897
                 IPCI
                       C14C0003-18; C14C0003-00 [C*]
                 IPCR C14C0003-00 [I,C*]; C14C0003-18 [I,A]
                NCL
                       008/094.330; 008/094.190R
                 ECLA
                      C14C003/18
     Hides or leather were tanned or retanned, resp., by treatment with an aqueous
AB
     bath containing a methylolated hydrophilic oligourethane with mol. weight
     300-20,000 and, optionally, HCHO or a HCHO-forming substance. Thus, 400 g
     nonaethylene glycol (1 mole) was dehydrated and mixed at 70° with
     151 g 1,6-hexamethylene diisocyanate (0.9 mole), and the mixture was heated
     to 120° over 1 hr and stirred another 5 hr at this temperature After the
     addition of 5 ml dimethylaminoethanol [108-01-0], the ir spectrum
     showed no NCO band. Dropwise addition of 1285 ml H2O gave a 30% solution of
     oligourethane [58043-06-4] with pH 7.5. This solution (100 g) was mixed with
     3.3 g of a 30% aqueous HCHO solution A chrome-tanned cowhide leather was
     neutralized to pH 4.5 with 1% Ca formate solution and treated 3 hr
     at 20° with a 3% aqueous solution of the above mixture to pH 4.3, a somewhat
     fuller, clear, soft leather resulted.
     oligourethane tanning hide leather
ΙT
     Urethane polymers, uses and miscellaneous
     RL: USES (Uses)
        (oligomeric, tanning with)
     Tanning
        (with olicourethanes)
     Poly(oxy-1,2-ethanediyloxy-1,2-ethanediyloxy-1,2-ethanediyloxy-1,2-
        ethanediyloxy-1,2-ethanediyloxy-1,2-ethanediyloxy-1,2-ethanediyloxy-1,2-
        ethanediyloxycarbonylimino-1,6-hexanediyliminocarbonyl), methanol
        blocked
     RL: USES (Uses)
        (oligomeric, tanning with)
     3,6,9,12,15,18,21-Heptaoxatricosane-1,23-diol, polymer with
        1,6-diisocyanatohexane, methanol-blocked
     Hexane, 1,6-diisocvanato-, polymer with
        3,6,9,12,15,18,21-heptaoxatricosane-1,23-diol, methanol-blocked
     RL: USES (Uses)
        (oligomeric, tanning with formaldehyde-containing)
     108-01-0D, Ethanol, 2-(dimethylamino)-, reaction products with
     polyurethanes
                   58043-08-6D, Poly(oxy-1,2-ethanediyloxy-1,2-ethanediyloxy-
     1,2-ethanediyloxy-1,2-ethanediyloxy-1,2-ethanediyloxy-1,2-ethanediyloxy-
     1,2-ethanediyloxy-1,2-ethanediyloxy-1,2-ethanediyloxycarbonylimino-1,6-
     hexanedivliminocarbonvl), reaction products with
                          58189-99-4D, Hexane, 1,6-diisocyanato-,
     dimethylaminoethanol
     polymer with 3,6,9,12,15,18,21-heptaoxatricosane-1,23-diol, reaction
     products with dimethylaminoethanol 58189-99-4D,
     3,6,9,12,15,18,21-Heptaoxatricosane-1,23-diol, polymer with
     1,6-diisocvanatohexane, reaction products with
     dimethylaminoethanol
     RL: USES (Uses)
        (oligomeric, tanning with)
     58043-06-4D, Hexane, 1,6-diisocyanato-, polymer with
     3,6,9,12,15,18,21,24-octaoxahexacosane-1,26-diol, reaction products with
     dimethylaminoethanol
                           58043-06-4D,
     3,6,9,12,15,18,21,24-Octaoxahexacosane-1,26-diol, polymer with
     1,6-diisocyanatohexane, reaction products with
     dimethylaminoethanol
                          58213-23-3
     RL: USES (Uses)
        (oligomeric, tanning with formaldehyde-containing)
1.9
    ANSWER 41 OF 55 CAPLUS COPYRIGHT 2009 ACS on STN
    1976:61229 CAPLUS
AN
DN
   84:61229
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OREF 84:10089a,10092a

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ED Entered STN: 12 May 1984
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- Leather tanning with oligourethanes
- Traeubel, Harro; Reiff, Helmut TN
- Bayer A.-G., Fed. Rep. Ger. PA
- SO Ger. Offen., 13 pp. CODEN: GWXXBX
- DT Pat ent.
- LA German
- IC C14C
- CC 41-3 (Leather and Related Materials)

KIND DATE

FAN.CNT 2 PATENT NO.

BR 7502008

US 4106897

DT DD 044	6.405		10051016	PR 1074 0416405	
	6485			DE 1974-2416485	
	6743			FR 1975-10657	19750327
FR 226	6743	B1	19781215		
DD 117	477	A5	19760112	DD 1975-185180	19750402
GB 149	5598	A	19771221	GB 1975-13397	19750402
BR 750	2008	A	19761221	BR 1975-2008	19750403
US 410	6897	A	19780815	US 1976-718489	19760830
PRAI DE 197	4-2416485	A	19740404		
DE 197	5-2504081	A	19750131		
IIS 197	5-561809	A2	19750325		
CLASS	3 301003	112	13730323		
	22 7 7 2	DATEME	EDMILY CLAC	SIFICATION CODES	
PATENT NO.		FAIENI	PARTET CEAS	SIFICATION CODES	
DE 2416485		C14C			
DE 2410400	IPCI		10 ITOM1.	C14C0003-16 [ICS]; C	1400003 00
	IFCI	(ICS,C		C14C0003-16 [1C5]; C	1400002-00
	IPCR			; C14C0003-18 [I,A]	
				; C14C0003-18 [1,A]	
	ECLA	C14C003			
FR 2266743	IPCI	C14C000	03-18 [ICM];	C14C0003-00 [ICM,C*]	
DD 117477	IPCI	C14C000	03-18 [ICM];	C14C0003-00 [ICM,C*]	
	IPCR	C14C000	03-00 [I,C*]	; C14C0003-18 [I,A]	
	ECLA	C14C003	3/18		
GB 1495598				C14C0003-16 [ICS]; C	1400003-00
05 1430030	1101			-06 [ICS]; C08G0018-0	
		[100,0	1, 00000010	_00 [ICD], C00G00IO_0	0 [100,0]

APPLICATION NO.

DATE

IPCR C14C0003-00 [I,C*]; C14C0003-18 [I,A] 008/094.330: 008/094.190R ECLA C14C003/18 Hides or leather were tanned or retanned, resp., with an aqueous liquor containing

methylolated oligourethanes with terminal OH groups and a mol. weight of 500-20,000 and HCHO or a HCHO-forming substance. Thus, 400 g nonaethylene glycol was dried and mixed at 70° with 151 g 1,6-hexamethylenediisocyanate, the mixture was heated to 120° in 1 hr

C14C0003-00 [I,C*]; C14C0003-18 [I,A]

C14C0003-00 [I,C*]; C14C0003-18 [I,A] C14C0003-18; C14C0003-00 [C*]

C14C0003-18 [ICM]; C14C0003-00 [ICM, C*]

and stirred another 5 hr at that temperature, 5 ml. of dimethylaminoethanol was added followed dropwise by 1285 ml H2O to

give a 30% oligourethane [58043-06-4] solution with pH 7.5. To 100 g of this solution was added 3.3 g of a 30% aqueous HCHO solution A chrome tanned

leather was neutralized with a 1% Ca formate solution to pH 4.5 and then processed 3 hr at 20° with the above product diluted to a 3% solids content with 10-fold H2O at a pH of 4.3. The process produced a somewhat fuller, softer retanned leather.

ST polyurethane tanning hide leather

IPCR

IPCI

IPCR

IPCI

NCL

Urethane polymers, uses and miscellaneous RL: USES (Uses)

```
(tanning with)
    Tanning materials
       (urethane polymers as)
    Tanning
       (with urethane polymers)
    58043-06-4 58043-08-6 58090-46-3 58189-99-4 58213-23-3
     RL: USES (Uses)
       (tanning with)
   ANSWER 42 OF 55 CAPLUS COPYRIGHT 2009 ACS on STN
AN 1974:426272 CAPLUS
DN 81:26272
OREF 81:4245a,4248a
ED Entered STN: 12 May 1984
TI Aminioorthesters as polvurethane catalysts
IN Bechara, Ibrahim S.; Holland, Dewey G.
SO U.S., 6 pp.
    CODEN: USXXAM
DT
   Patent
LA
   English
TC
    C08G
INCL 260075000NC
   35-4 (Synthetic High Polymers)
FAN.CNT 2
    PATENT NO.
                       KIND
                              DATE
                                          APPLICATION NO.
                        A 19740115 US 1972-276976
A 19750422 US 1973-393722
B 19810306 JP 1973-135424
    US 3786029
    US 3879465
                                                                 19730904
    JP 56010301
                        A3
PRAI US 1972-276976
                              19720801
CLASS
PATENT NO. CLASS PATENT FAMILY CLASSIFICATION CODES
US 3786029
               IC C08G
                INCL 260075000NC
                IPCI C08G0022-38 [ICM]; C08G0022-46 [ICS]
                NCL
                       528/053.000; 521/129.000; 521/172.000; 521/178.000;
                       528/044.000; 528/051.000; 528/072.000; 528/076.000;
                       528/080.000; 564/346.000; 564/434.000; 564/504.000;
                       564/505.000
US 3879465
                IPCI C07C0093-02 [ICM]
                IPCR C08G0018-00 [I.C*]; C08G0018-18 [I.A]; C08G0059-00
                       [I.C*1: C08G0059-50 [I.A]
                NCL
                       564/504.000; 521/129.000; 564/346.000
                ECLA C08G018/18G; C08G059/50H
JP 56010301
                IPCI C07C0093-04 [ICM]; C08G0018-18 [ICA]; C08G0018-00
                       [ICA,C*]
    Aminoorthoesters with good stability, low odor and toxicity, useful as
     polyurethane catalysts and curing agents for epoxy resins, were prepared
     from aminoalkanols and orthoesters RC(OR1)3 (R = H, Ph, C1-4 alkyl, R1 =
     C2-4 alkyl). Thus, a mixture of Me orthoformate [149-73-5] 10.6, 2-(
     dimethylamino)ethanol (I) [108-01-0] 27 and p-MeC6H4SO3H
     0.3 g was refluxed for several days and distilled, to obtain two fractions
     at 95-100.deg./3 mm and 135.deg./3 mm which were identified as methoxy
     bis(diethylaminoethyl)formate [51877-55-5] and
     tris(diethylaminoethyl)formate (II) [51936-97-1] resp. A
    urethane foam composition containing polyol 109, blowing agent 47, surfactant
1.5,
     di-Bu tin dilaurate 0.12, diisocyanate 105 and II 0.8 g showed gel time 35
    sec, rise time 63 sec and tack free time 47 sec as compared with 118, 265
```

ST aminoester polyurethane foam catalyst; ester amino polyurethane catalyst

and 222 for a similar compn containing I.

```
Esters, uses and miscellaneous
     RL: PREP (Preparation)
         (aminoortho-, catalysts, for polyurethane foam preparation)
     Polymerization catalysts
      (aminoorthoesters, for polyurethane foam manufacture)
     Urethane polymers, preparation
     RL: PREP (Preparation)
         (cellular, aminoorthoester catalysts for)
     38565-71-8P 38565-72-9P 51936-97-1P 52379-12-1P 52379-13-2P 52379-14-3P 52379-15-4P 52379-16-5P 52379-17-6P 52379-18-7P
     RL: PREP (Preparation)
        (preparation of)
ΙT
     78-39-7 122-51-0 149-73-5
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (reaction of, with aminoalkanols)
     100-37-8 108-16-7 1704-62-7 5966-51-8
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (reaction of, with orthoesters)
L9
     ANSWER 43 OF 55 CAPLUS COPYRIGHT 2009 ACS on STN
    1974:134171 CAPLUS
AN
DN
    80:134171
OREF 80:21641a,21644a
ED Entered STN: 12 May 1984
    Storage-stable polyols for polyurethane foams
    Crawshaw, Robert A.; Loible, John E.; Moffatt, Vivian A.
TN
    Shell Internationale Research Maatschappij N. V.
SO Ger. Offen., 15 pp.
    CODEN: GWXXBX
DT
    Patent
    German
LA
IC.
    C08G
     36-2 (Plastics Manufacture and Processing)
FAN.CNT 1
     FAIENT NO. KIND DATE
                                              APPLICATION NO.
                                                                       DATE
                         A1 19731115 DE 1973-2321884
A 19740508 DF 1973-48261
B 19810108
A1 19731214 FR 1973-15385
A1 19731030 BE 1973-130593
A 19741031 AU 1973-54986
B 19750430 II 1973-23568
                                                                      19730430
PΙ
    DE 2321884
     JP 49047495
JP 56000446
     FR 2183072
                                                                        19730427
     BE 798926
                                                                       19730430
     AU 7354986
                                                                       19730430
     IT 988642
                                                                        19730430
11 988042 B 1970430 I 1973-22566
AIT 7303823 A 19751015 AIT 1973-3823
AIT 331034 B 19760726
CH 592122 A5 19771014 CH 1973-6129
NL 7306021 A 19731106 NL 1973-6021
PRAI GB 1972-20357 A 19720502
                                                                        19730430
                                                                       19730430
                                                                        19730501
CLASS
 PATENT NO. CLASS PATENT FAMILY CLASSIFICATION CODES
                  IC C08G
 DE 2321884
                  IPCI C08G0022-44 [ICM]
                  IPCR C08G0018-00 [I,C*]; C08G0018-00 [I,A]; C08G0018-42
                         [I,A]; C08G0065-00 [I,C*]; C08G0065-26 [I,A];
                         C08J0009-00 [I,C*]; C08J0009-00 [I,A]
                  ECLA C08G065/26P3C; C08J009/00R+L75/08
 JP 49047495
                  IPCI C08G0022-14
                  TPCR
                         C08G0018-00 [I,C*]; C08G0018-00 [I,A]; C08G0018-42
                         [I,A]; C08G0065-00 [I,C*]; C08G0065-26 [I,A];
                         C08J0009-00 [I,C*]; C08J0009-00 [I,A]
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TPCR
                       C08G0018-00 [I,C*]; C08G0018-00 [I,A]; C08G0018-42
                        [I,A]; C08G0065-00 [I,C*]; C08G0065-26 [I,A];
                        C08J0009-00 [I,C*]; C08J0009-00 [I,A]
                 ECLA
                       C08G065/26P3C; C08J009/00R+L75/08
 BE 798926
                 IPCI
                       COSG [ICM]
                 IPCR
                       C08G0018-00 [I,C*]; C08G0018-00 [I,A]; C08G0018-42
                       [I,A]; C08G0065-00 [I,C*]; C08G0065-26 [I,A];
                        C08J0009-00 [I,C*]; C08J0009-00 [I,A]
                 IPCI
AU 7354986
                       C08G0022-46 [ICM]
                 IPCR
                       C08G0018-00 [I,C*]; C08G0018-00 [I,A]; C08G0018-42
                       [I,A]; C08G0065-00 [I,C*]; C08G0065-26 [I,A];
                        C08J0009-00 [I,C*]; C08J0009-00 [I,A]
                 ECLA
                       C08G065/26P3C; C08J009/00R+L75/08
 TT 988642
                 TPCT
                       C08G [ICM]
                 TPCR
                       C08G0018-00 [I,C*]; C08G0018-00 [I,A]; C08G0018-42
                       [I,A]; C08G0065-00 [I,C*]; C08G0065-26 [I,A];
                        C08J0009-00 [I,C*]; C08J0009-00 [I,A]
                 ECLA
                       C08G065/26P3C; C08J009/00R+L75/08
AT 7303823
                 IPCI
                       C08L0075-08 [ICM]; C08L0075-00 [ICM,C*]; C08K0005-09
                        [ICS]; C08K0005-00 [ICS,C*]; C08J0009-00 [ICS]
                 IPCR
                       C08G0018-00 [I,C*]; C08G0018-00 [I,A]; C08G0018-42
                        [I,A]; C08G0065-00 [I,C*]; C08G0065-26 [I,A];
                        C08J0009-00 [I,C*]; C08J0009-00 [I,A]
                 ECLA
                       C08G065/26P3C: C08J009/00R+L75/08
CH 592122
                 IPCI
                       C08G0018-48 [ICM]; C08G0018-00 [ICM,C*]
                 TPCR
                       C08G0018-00 [I,C*]; C08G0018-00 [I,A]; C08G0018-42
                        [I,A]; C08G0065-00 [I,C*]; C08G0065-26 [I,A];
                       C08J0009-00 [I,C*]; C08J0009-00 [I,A]
                 ECLA
                       C08G065/26P3C; C08J009/00R+L75/08
NL 7306021
                 IPCI
                       C08G0022-14 [ICM]
                 IPCR
                       C08G0018-00 [I,C*]; C08G0018-00 [I,A]; C08G0018-42
                       [I,A]; C08G0065-00 [I,C*]; C08G0065-26 [I,A];
                       C08J0009-00 [I,C*]; C08J0009-00 [I,A]
                 ECLA
                       C08G065/26P3C; C08J009/00R+L75/08
    Polyurethane foams containing homogenous closed cells, useful for refrigerator
AB
     linings, were prepared by mixing of storage- and heat-stable polyols
     stabilized by formic acid [64-18-6] and polyisocyanates. Thus,
     a mixture containing sucrose 273, propylene oxide 655, ethylene oxide 72, and
     dimethylaminoethanol catalyst 3.0 kg reacted at 90.deg. to give a
     polvol (I) of mol. weight 1200, OH number 400 mg KOH/g, pH 11.4 (25% agueous
solution)
     to which 1.58 kg agueous 98% HCO2H was added to adjust pH to 7.3. A mixture
     (100 parts) containing I 70, polyol (from glycerol and propylene oxide) 30,
     silicone oil (DC 193) 1, Dabco 33 LV (triethylenediamine) 0.5, Dime 6
     (N,N-dimethylcyclohexylamine) 2, and H2O 2 parts, kept 24 hr at 50.deg.,
     was treated with 120 parts diisocvanatodiphenylmethane and 30 parts CFC13
     foaming agent to give a foam of content of closed cells 81.8 volume% and
     heat conductivity (Btu in./ft2/hr/degree F) 0.170, compared with 83.3 and 0.164
     for a foam prepared from HCO2H-stabilized I after 0 hr storage. Foams
     prepared similarly from I containing no HCO2H had 92.8 and 50.4 volume % closed
    cells, resp., and heat conductivity 0.157 and 0.530, resp., when the I was
```

0 and 24 hr at 50.deg, before use.

stabilizer formic acid polyol; polyurethane foam insulation;

sucrose polyol heat stabilizer; heat insulation polyurethane foam Urethane polymers, preparation

RL: PREP (Preparation)

(cellular, with closed cells, heat-stabilized polyols for) Heat stabilizers

(formic acid, for polyols, in polyurethane manufacture)

IT Thermal insulation

```
(polyurethane foams, with closed cells)
    64-18-6, uses and miscellaneous
    RL: MOA (Modifier or additive use); USES (Uses)
        (heat stabilizers, for polyols, for polyurethane foam with closed
       cells)
   ANSWER 44 OF 55 CAPLUS COPYRIGHT 2009 ACS on STN
L9
AN
    1973:45227 CAPLUS
DN
    78:45227
OREF 78:7141a,7144a
ED Entered STN: 12 May 1984
TΙ
   Applying a cast polyurethane layer to the surface of a polyamide molding
IN
    Veres, Ladislaus
PA
   Kabel- und Metallwerke Gutehoffnungshuette A.-G.
SO
    Ger., 4 pp.
    CODEN: GWXXAW
DT
    Patent
LA
    German
IC
    B44D
    42-10 (Coatings, Inks, and Related Products)
FAN.CNT 1
    PATENT NO.
                      KIND
                             DATE
                                        APPLICATION NO.
                              ----
     -----
                       ----
                                         -----
                                       DE 1971-2142970
                                                              19710827
PΤ
    DE 2142970
                       A
                             19720831
    DE 2142970
                       В
                              19720831
                       C2 19730405
    DE 2142970
PRAI DE 1971-2142970
                       A
                              19710827
CLASS
PATENT NO.
              CLASS PATENT FAMILY CLASSIFICATION CODES
 ------
              IC B44D
DE 2142970
                IPCI B44D0001-22
AB
    Cast polyurethane elastomer was bonded to a polyamide molding by
    pretreating the polyamide molding with a formic acid
    [64-18-6]-\beta-(dimethylamino)ethanol(I)[108-01-0]
    mixture with the end of the reaction between HCO2H and I indicated by methyl
    red. Thus, the circumference of a polyamide wheel was sprayed with a 1:10
    HCO2H-HCO2Me solution containing a drop of methyl red and further sprayed with
а
    1:10 I-CHC13 solution until the color of the indicator disappeared to give a
    coated wheel which was molded with a rubbery polyurethane mass to form a
    polyurethane rim strongly bonded to the polyamide wheel.
ST
    formate adhesive polyamide; aminoethanol ester adhesive;
    polyurethane polyamide adhesion
    Adhesives
        ((dimethylamino)ethanol-formic acid, for
       bonding of polyurethane rubber on polyamide wheels)
    Rubber, urethane, uses and miscellaneous
       (casting of, on polyamide wheels, formic acid-(
       dimethylamino)ethanol adhesives for)
    Molding of plastics and rubbers
       (of urethane rubber, on polyamide wheels, formic acid-(
       dimethylamino)ethanol adhesives for)
    Polyamides, uses and miscellaneous
    RL: USES (Uses)
        (wheels, bonding of polyurethane rubber on, adhesives for)
    64-18-6, uses and miscellaneous
    RL: USES (Uses)
        (adhesives, containing (dimethylamino)ethanol, for
       bonding polyurethane rubber to polyamide wheels)
    108-01-0
    RL: USES (Uses)
```

(adhesives, containing formic acid, for bnding polyurethane rubber to polyamide wheels)

- ANSWER 45 OF 55 CAPLUS COPYRIGHT 2009 ACS on STN 1.9 AN 1966:482135 CAPLUS DM 65:82135 OREF 65:15320f-g ED Entered STN: 22 Apr 2001 TI Synthesis of heterocyclic compounds. CLIV. Novel methylation. 3. Methylation of tertiary amines such as pyridine and isoquinoline with alkvl carboxvlates ΑU Kametani, Tetsuji; Kigasawa, Kazuo; Hayasaka, Tetsutaro; Hiiragi, Mineharu; Ishimaru, Haruhide; Asagi, Setsu CS School Med., Tohoku Univ., Sendai, Japan SO Journal of Heterocyclic Chemistry (1966), 3(2), 129-36 CODEN: JHTCAD; ISSN: 0022-152X DT Journal LA English 37 (Heterocyclic Compounds (One Hetero Atom)) AB cf. CA 63, 6911h; preceding abstract The alkylation of tertiary amines, namely, 2-dimethylaminoethanol, triethylamine, pyridine, and isoquinoline with various alkyl carboxylates was investigated. This reaction afforded the corresponding quaternary ammonium salts, e.g., methylation of 2-dimethylaminoethanol with methyl salicylate. Heterocyclic compounds Amines (alkylation of tertiary, with alkyl carboxylates) Methylation (of amines (tertiary) with Me carboxylates) Alkylation (of tertiary amines with alkyl carboxylates) 93-58-3 99-96-7 107-31-3 619-50-1 (Derived from data in the 7th Collective Formula Index (1962-1966)) 121-44-8, Triethylamine (alkylation by alkyl carboxylates) 108-01-0, Ethanol, 2-(dimethylamino)-(alkylation of) 110-86-1, Pyridine 119-65-3, Isoquinoline (methylation with alkyl carboxylates) 600-23-7P, Oxalic acid, methyl ester 606-45-1P, o-Anisic acid, methyl ester 2756-87-8P, Fumaric acid, methyl ester 3878-55-5P, Succinic
- (preparation of)

 11 610-34-4, Benzoic acid, o-nitro-, ethyl ester 615-98-5, Oxalic acid, dipropyl ester 2050-60-4, Oxalic acid, dibutyl ester 7579-36-4, Oxalic acid, dibenzyl ester 7579-38-6, Benzoic acid, o-nitro-, benzyl ester 7570-40-0, Benzoic acid, o-chloro-, benzyl ester (tertiary amine alkylation with)
- IT 62-23-7, Benzoic acid, p-nitro- 64-18-6, Formic acid 65-85-0, Benzoic acid 95-92-1, Oxalic acid, diethyl ester 99-76-3, Benzoic acid, p-hydroxy-, methyl ester 105-34-0, Acetic acid, cyano-, methyl ester 106-65-0, Succinic acid, dimethyl ester 108-59-8, Malonic acid, dimethyl ester 55-9-02, Cyalic acid, dimethyl ester 55-9-02, Oxalic acid, dimethyl ester 554-12-1, Propionic acid, methyl ester 606-27-9, Benzoic acid, o-nitro-, methyl ester 610-95-8, Benzoic acid, o-chloro-, methyl ester 618-95-1, Benzoic acid, m-nitro-, methyl ester 624-48-6, Maleic acid, dimethyl ester 624-49-7, Fumaric acid, dimethyl ester 4376-18-5, Phthalic acid, methyl ester

(tertiary amine methylation with)

acid, methyl ester RL: PREP (Preparation)

```
AN 1963:20566 CAPLUS
DN 58:20566
OREF 58:3360q-h
ED Entered STN: 22 Apr 2001
TI Isophthalic acid-ethyl carbonate dianhydride
IN Curtius, Ulrich; Boellert, Volker; Fritz, Gerhard; Nentwig, Joachim
PA Farbenfabriken Bayer A.-G.
SO 37 pp.
DT Patent
LA Unavailable
CC 35 (Noncondensed Aromatic Compounds)
FAN.CNT 1
     PATENT NO.
                       KIND DATE APPLICATION NO.
                                                                 DATE
                               19620515 BE
PΤ
   BE 616919
     DE 1210853
                                           DE
     FR 1334980
                                            FR
     GB 975368
                                            GB
PRAI DE
                                19610525
CLASS
 PATENT NO.
               CLASS PATENT FAMILY CLASSIFICATION CODES
   C1CO2Et is dissolved i 1 CH2C12, Me(C18H37)N(CH2)3OH added,
     m-C6H4(CO2H)2 neutralized with NaOH, the neutral solution poured into the
     solution of C1CO2ET, the mixture kept at 18-20° 20 min., the 2 phases
     separated, the aqueous phase exted. with CH2Cl2, and the CH2Cl2 solns.
combined.
     washed with H2O, dried, and evaporated to give m-C6H4(CO2CO2ET)2
     solidification point 23-4°. Other amines used as catalyst are
     MeN(n-C18H37)2, and Me3(C12H25N+C1-
    Amines
       (catalysts from tertiary, for dialkyl oxydiformate manufacture)
    Catalysts and Catalysis
        (for dialkyl oxydiformate manufacture, trialkylamines as)
     4455-26-9P, Dioctylamine, N-methyl- 99772-22-2P, Hexanamide,
     (dimethylamino)-N-dodecyl- 102960-93-0P, Undecanamide,
     (dimethylamino)-N-octadecyl-
     RL: PREP (Preparation)
        (as catalyst for dialkyl oxydiformate manufacture)
     108084-10-2, Hexanamide, (dimethylamino)-N-octadecyl-
        (as catalyst for dialkyl oxydiformates)
     112-18-5P, Dodecylamine, N, N-dimethyl- 124-28-7P, Octadecylamine,
     N, N-dimethyl- 4088-22-6P, Dioctadecylamine, N-methyl- 10182-91-9P,
     Ammonium, dodecyltrimethyl
     RL: PREP (Preparation)
        (catalysts, for dialkyl oxydiformate manufacture)
     1609-47-8P, Formic acid, oxydi-, diethyl ester 4525-32-0P,
     Formic acid, oxydi-, dibutyl ester 4525-33-1P, Formic
     acid, oxydi-, dimethyl ester 22483-52-9P, Isophthalic acid, dianhydride
     with EtHCO3 22483-52-9P, Carbonic acid, ethyl ester, dianhydride with isophthalic acid 94250-86-9P, Propionic acid, 3-(p-chlorophenoxy)-,
     2-(diethylamino)ethyl ester 94250-87-0P, Propionic acid,
     3-(p-chlorophenoxy)-, 2-(diethylamino)ethyl ester, hydrochloride
     RL: PREP (Preparation)
        (preparation of)
    75-21-8P, Ethylene oxide
     RL: PREP (Preparation)
        (reaction products of, with N-methyloctadecylamine, catalysts for
        dialkyl oxydiformate manufacture)
    75-56-9P, Propylene oxide
     RL: PREP (Preparation)
        (reaction products with 2-(dimethylamino)ethanol,
```

```
(reaction products with ethylene oxide, as catalysts for dialkyl
        oxydiformate manufacture)
     108-01-0P, Ethanol, 2-(dimethylamino) - 2439-55-6P, Octadecylamine,
     N-methyl-
     RL: PREP (Preparation)
        (reaction products with propylene oxide, as catalysts for dialkyl
       oxydiformate manufacture)
     75-56-9P, Propylene oxide
     RL: PREP (Preparation)
        (reaction products with N-methyloctadecylamine, as catalysts for
        dialkyl oxydiformate manufacture)
    ANSWER 47 OF 55 CAPLUS COPYRIGHT 2009 ACS on STN
1.9
ΔN
    1963:3344 CAPLUS
DN 58:3344
OREF 58:540a-h,541a-c,542a-c
    Entered STN: 22 Apr 2001
    Dihydrodibenzothiazepines
IN
    Yale, Harry L.; Sowinski, Francis A.
   Olin Mathieson Chemical Corp.
PA
SO
    8 pp.
   Patent
DT
    Unavailable
LA.
INCL 260293400
    38 (Heterocyclic Compounds (More Than One Hetero Atom))
FAN.CNT 1
    PATENT NO.
                                                                DATE
                      KIND DATE
                                        APPLICATION NO.
                        ----
                                          -----
    US 3050524
                              19620821 US
                                                                19610210
    FR 1318032
                                          FR
                                          FR
     FR M2074
     GB 993529
                                           GB
PRAI US
                               19610210
CLASS
PATENT NO. CLASS PATENT FAMILY CLASSIFICATION CODES
               INCL 260293400
                NCL
                       540/547.000; 250/396.000R; 564/184.000; 564/221.000;
                       564/418.000; 564/422.000; 564/430.000; 568/044.000
O.S.
    MARPAT 58:3344
AB
    The appropriate o-chloronitrobenzene was refluxed with a suitable
     benzenethiol in the presence of NaOH to obtain the corresponding
     2-nitrophenyl Ph sulfide, reduced with nascent hydrogen to the
     2-(phenylthio)aniline derivative This was treated with formic acid
     to obtain the 2-(phenylthio) formanilide or with an alkanovl halide to
     obtain an 11-unsubstituted product or with an arylcarbonyl halide to
    obtain an II-substituted product. Treatment with a mixture of
     polyphosphoric acid and phosphorus oxychloride yielded a
    dibenzo[b,f]-1,4-thiazepine, reduced with a mixture of LiAlH4 and AlC13 to
     the corresponding 10,11-dihydrodibenzo[b,f]-1,4-thiazepine; its
     10-carbonyl chloride (I) was obtained by treatment with phosgene. Certain
     of the compds. were useful ataractic agents. Thus, 44 g. NaOH in 100 mL.
     water was added to 211 g. 2,5-dichloronitrobenzene and 110.2 g.
     benzenethiol in 500 mL. 95% ethanol and the mixture refluxed 2.5 h. to yield
     280.4 g. crude 4-chloro-2-nitrophenyl Ph sulfide (III), m. 83-4°
     (95% ethanol). To 265.7 g. III, 558 g. iron powder, and 2 1. 95% ethanol
    was added dropwise 25 mL. concentrated HCl. After the spontaneous reaction had
    subsided, which occurred on heating the mixture to 55°, the mixture was
     refluxed 3 h., filtered, and the filtrate concentrated to give 227 g. crude
```

as catalysts for dialkyl oxydiformate manufacture)

2439-55-6P, Octadecylamine, N-methyl-

RL: PREP (Preparation)

```
5-chloro-2-(phenylthio)aniline (IV), m. 62-3°. Treatment with dry
     HCl in anhydrous ether gave IV hydrochloride, m. 164-6°. A mixture of
     221.7 g. III, 460 g. 98% formic acid, and 102.1 g. acetic
     anhydride was refluxed one hr., concentrated in vacuo, and the residue poured
on
     ice to yield 244 g. 5-chloro-2-(phenylthio)formanilide (V), m.
     55-6° (benzene-ligroine). Being careful to control foaming, a well
     blended mixture of 50.0 q. V, 400 q. polyphosphoric acid, and 58.3 q.
     phosphorus oxychloride was heated 1.5 h. at 120-3° under nitrogen
     using an ore bath. On cooling, the mixture was treated with crushed ice,
    made strongly alkaline with concentrated ammonia, and extracted with ether.
The concentrated
     ether extract gave 53.7 g. crude 8-chlorodibenzo[b,f]-1,4-thiazepine (VI), m.
     78-9° (hexane). To 3.9 g. LiAlH4 and 13.3 g. AlC13 in 100 mL. dry
     ether was added dropwise 12.3 g. VI in 100 mL. dry ether, which upon work
     up yielded 12.6 g. crude 8-chloro-10,11-dihydrodibenzo[b,f]-1,4-thiazepine
     (VII), m. 126-7° (95% ethanol).
     10,11-Dihydro-8-(trifluoromethyl)dibenzo[b,f]-1,4-thiazepine, m.
     99-100°, was similarly prepared using
     phenyl-a, a, a-trifluoro-2-nitro-p-tolyl sulfide, m.
     70-1° (absolute ethanol), α,α,α-trifluoro-6-
     (phenylthio)m-formotoluidide, m. 55-6° (ligroine), and
     8-(trifluoromethyl)dibenzo[b,f]-1,4-thiazepine, m. 83-4°
     (ligroine). 10.11-Dihydrodibenzo[b.f]-1.4-thiazepine was similarly prepared
     using 2-nitrodiphenyl sulfide, m. 77-8°.
     2,8-Dichloro-10,11-dihydrodibenzo[b,f]-1,4-thiazepine was similarly prepared
     To 4.8 g. NaOH in 50 mL. water at 0° was added 9.0 g.
     o-(phenylthio)aniline, 25 mL. benzene, and 5.9 g. benzoyl chloride. The
     mixture was shaken one hr. and the benzene solution worked up to yield 9 g.
     2-(phenylthio)benzanilide, m. 69-70° (95% ethanol). Following the
     procedure for VI, 11-phenyldibenzo[b,f]-1,4-thiazepine (VIII), m.
     110-11°, was obtained. To 9.3 g. anhydrous AlCl3 and 2.66 g. LiAlH4
     in 250 mL. anhydrous Et20 was added 10 q. VIII in 200 mL. anhydrous Et20, after
     stirring one hr. and refluxing one more hr. the excess reducing agent
     destroyed, and the mixture worked up to yield 9 q.
     10,11-dihydro-11-phenyldibenzo[b,f]-1,4-thiazepine, m. 105-6°.
     Similarly prepared were: 10,11-dihydro-11-methyldibenzo[b,f]-1,4-thiazepine;
     10,11-dihydro-8-chloro-11-phenyldibenzo[b,f]-1,4-thiazepine; and
     10,11-dihydro-8-(trifluoromethyl)-11-phenyldibenzo[b,f]-1,4-thiazepine.
     To a stirred solution of 20.0 g. VII in 150 mL. dry toluene cooled to
     -10° was added 170 mL. 9.3% toluene solution of phosgene (also cooled
     to -10°) then immediately 7.1 g. pyridine. The mixture was stirred 3
     h., allowed to stand overnight, filtered, washed with water, dried over
     anhydrous MgSO4, and concentrated to give 16.3 g. 8-chloro-10,11-dihydrodibenzo
     [b,f]-1,4-thiazepine-10-carbonyl chloride (IX), m. 114-15°
     (Skellysolve V). Similarly prepared were:
     8-(trifluoromethyl)-10,11-dihydrodibenzo[b,f]-1,4-thiazepine-10-carbonyl
     chloride, m. 94-6°: 10,11-dihydrodibenzo(b.f]-1,4-thiazepine-10-
     carbonyl chloride, m. 114-15° (Skellysolve V);
     2,8-dichloro-10,11-dihydrodibenzo[b,f]-1,4-thiazepine-10-carbonyl
     chloride; 10,11-dihydro-11-phenyldibenzo[b,f]-1,4-thiazepine-10-carbonyl
     chloride; 10,11-dihydro-11-methyldibenzo[b,f]-1,4-thiazepine-10-carbonyl
     chloride; 10,11-dihydro8-chloro-11-phenyldibenzo[b,f]-1,4-thiazepine-10-
     carbonyl chlorine; 10,11-dihydro-8-(trifluoromethyl)-11-
     phenyldibenzo[b,f]1,4-thiazepine-10-carbonyl chloride. A mixture of 5.0 g.
     IX, 14.3 g. dimethylaminoethanol, and 150 mL. solvent was
     refluxed 5 h., the supernatant decanted, and worked up to yield 2.2 g.
     8-chloro-10,11-dihydrodibenzo[b,f]-1,4-thiazepine-10-carboxylic acid;
     ester with 2-dimethylaminoethanol (X) m. 86-70
     (ligroine). Similarly prepared were:
     10,11-dlhydro-8-(trifluoromethyl)dibenzo[b,f]-1,4-thiazepine-10-carboxylic
     acid ester of 2-dimethylaminoethanol, m. 76.5-7.5°;
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```
2,8-dichloro-10,11-dihydrodibenzo[b,f]-1,4-thiazepine-10-carboxylic acid
ester of 2-dimethylaminoethanol;
10,11-dihydrodibenzo[b,f]-1,4-thiazepine-10-carboxylic acid ester of 2-
dimethylaminoethanol (XI) in the presence of 50% NaH-mineral oil;
2,8-dichloro-10,11-dihydrodibenzo[b,f]-1,4-thiazepine-10-carboxylic acid
ester of 2-dimethylaminoethanol;
10,11-dihydro-11-phenyldibenzo[b,f]-1,4-thiazepine-10-carboxylic acid
ester of 2-dimethylaminoethanol;
10,11-dihydro-11-methyldibenzo[b,f]-1,4-thiazepine-10-carboxylic acid
ester of 2-diethylaminoethanol; 10,11-dihydro-8-chloro-11-
phenyldibenzo[b,f]-1,4-thiazepine-10-carboxylic acid ester of 2-
dimethylaminoethanol; and 10,11-dihydro-8-(trifluoromethyl)-11-
phenyldibenzo[b,f]-1,4-thiazepine-10-carboxylic acid ester of 2-
dimethylaminoethanol. To a cooled solution 11.3 g. XI in 100 mL.
anhydrous Et20 was added in small portions 5.0 g. maleic acid in 40 mL.
acetone to yield 10.3 g. 10,11-dihydrodibenzo[b,f]-1,4-thiazepine-10-
carboxylic acid ester of 2-dimethylaminoethanol monomaleic acid
salt, m. 108-10°. A mixture of 10.3 g. IX, 17.3 g.
2-(2-piperidinoethoxy)ethanol, and 150 mL. dry toluene was refluxed. 7 h.
and worked up to give 7.8 g. 8-chloro-10,11-dihydrodibenzo[b,f]-1,4-
thiazepine-10-carboxylic acid ester of 2-(2-piperidinoethoxy)ethanol
(XII). To 7.8 g. XII in 100 mL, anhydrous Et20 was added 1.6 g. oxalic acid
in 10 mL, acetone, left standing in Et20 several days, and worked up to
give 3.7 g. 8-chloro-10,11-dihydrodibenzo[b,f]-1,4-thiazepine-10-
carboxylic acid ester of 2-(2-piperidinoethoxy)ethanol monooxalic acid
salt, m. 99-100° (Me Et ketone). Similarly prepared were:
8-(trifluoromethyl)-10,11-dihydrodibenzo[b,f]-1,4-thiazepine-10-carboxylic
acid ester of 2-(2-piperidinoethoxy)ethanol monooxalic acid salt, m.
104-6°; 10,11-dihydrodibenzo[b,f]-1,4-thiazepine-10-carboxylic acid
ester of 2-(2-piperidinoethoxy)ethanol monooxalic acid salt, tn.
141-2° (absolute ethanol); 8-chloro-10,11-dihydrodibenzo[b,f]-1,4-
thiazepine-10-carboxylic acid ester of 3-(4-methylpiperazino)propanol
hydrochloride. A mixture of 10.3 g. IX, 8.9 g. 2-dimethylaminoethylamine,
and 150 mL. dry toluene was refluxed 5 h. and worked up using the
procedure for V to give 8-chloro-10,11-dihydrodibenzo[b,f]-1,4-thiazepine-
10-carboxylic acid 2-dimethylaminoethylamide. Similarly prepared were:
10,11-dihydro-8-(trifluoromethyl)dibenzo[b,f]-1,4-thiazepine-10-carboxylic
acid 2-dimethylaminoethylamide; 10,11-dihydrodibenzo[b,f]-1,4-thiazepine-
10-carboxylic acid 2-dimethylaminoethylamide;
10,11-dihydrodibenzo[b,f]-1,4-thiazepine-10-carboxylic acid
2-dimethylaminoethylamide; 2,3-dichloro-10,11-dihydrodibenzo[b,f]-1,4-
thiazepine-10-carboxylic acid 2-dimethylaminoethylamide;
10,11-dihydrophenyldibenzo[b,f]-1,4-thiazepine-10-carboxylic acid
2-dimethylaminoethylamide; 10,11-dihydro-11-methyldibenzo[b,f]-1,4-
thiazepine-10-carboxylic acid 2-diethylaminoethylamide;
10,11-dihydro-8-chloro-11-phenyldibenzo[b,f]-1,4-thiazepine-10-carboxylic
acid 2-dimethylaminoethylamide; 10,11-dihydro-8-(trifluoromethyl)-11-
phenyldibenzo[b,f]-1,4-thiazepine-10-carboxylic acid
2-dimethylaminoethylamide; and 8-chloro-10,11-dihydrodibenzo[b,f]-1,4-
thiazepine-10-carboxylic acid 2-(2-piperidinoethoxy)-ethylamide (X). To
4.46 q. X in 100 mL. anhydrous Et20 was added a warm solution of 0.9 q. oxalic
acid in 10 mL. acetone to yield 8-chloro-10,11-dihydrodibenzo[b,f]-1,4-
thiazepine-10-carboxylic acid 2-(2-piperidinoethoxy)ethylamide monooxalic
acid salt. Similarly prepared was 8-chloro-10,11-dihydrodibenzo[b,f]-1,4-
thiazepine-10-carboxylic acid 3-(4-methylpiperazino)propylamide
hydrochloride.
1580-66-1
            7586-09-6
                       36599-14-1
   (Derived from data in the 7th Collective Formula Index (1962-1966))
109806-80-6P
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RL: SPN (Synthetic preparation); PRP (Properties); PREP (Preparation)

3603-43-8, Ethanol, 2-(2-piperidinoethoxy)- 5317-33-9,

(Dihydrodibenzothiazepines)

```
1-Piperazinepropanol, 4-methyl-
   (esters)
346-44-1P, Sulfide, phenyl a,a,a-trifluoro-2-nitro-p-
      735-73-9P, m-Formotoluidide,
α,α,α-trifluoro-6'-(phenylthio)-
                                 790-17-0P.
Dibenzo[b,f][1,4]thiazepine, 10,11-dihydro-8-(trifluoromethyl)-
802-19-7P, Dibenzo[b,f][1,4]thiazepine,
10,11-dihydro-11-phenyl-8-(trifluoromethyl)- 1489-18-5P,
Dibenzo(b, f)[1, 4]thiazepine, 10,11-dihvdro-11-phenvl- 1489-19-6P,
Dibenzo[b,f][1,4]thiazepine, 10,11-dihydro-11-methyl-
Dibenzo[b,f][1,4]thiazepine, 11-phenyl- 1545-76-2P,
Dibenzo[b,f][1,4]thiazepine, 8-(trifluoromethv1)-
                                                  1647-55-8P.
Dibenzo[b,f][1,4]thiazepine-10(11H)-carboxamide,
N-[2-(dimethylamino)ethyl]-8-(trifluoromethyl)-
                                                2558-02-3P,
Dibenzo[b,f][1,4]thiazepine-10(11H)-carboxylic acid, 8-(trifluoromethyl)-,
2-(2-piperidinoethoxy)ethyl ester, oxalate 2729-83-1P,
Dibenzo[b,f][1,4]thiazepine-10(11H)-carboxylic acid, 8-(trifluoromethyl)-,
2-(dimethylamino)ethyl ester
                             2926-88-7P,
Dibenzo[b, f][1,4]thiazepine-10(11H)-carbonyl chloride,
8-(trifluoromethyl) - 3526-11-2P, Benzanilide, 2'-(phenylthio)-
3798-57-0P, Dibenzo[b,f][1,4]thiazepine-10(11H)-carboxylic acid,
11-phenyl-8-(trifluoromethyl)-, 2-(dimethylamino)ethyl ester 4171-83-9P,
Sulfide, o-nitrophenyl phenyl 4177-88-2P, Aniline,
5-chloro-2-(phenylthio)-, hydrochloride
                                        4177-89-3P, Formanilide,
5'-chloro-2'-(phenylthio)- 4177-90-6P, Dibenzo[b,f][1,4]thiazepine,
          4177-91-7P, Dibenzo[b,f][1,4]thiazepine,
8-chloro-
8-chloro-10,11-dihydro- 4235-20-5P, Aniline, 5-chloro-2-(phenylthio)-
4548-56-5P, Sulfide, 4-chloro-2-nitrophenyl phenyl 4573-64-2P,
Dibenzo(b, f)(1,4)thiazepine-10(11H)-carboxamide,
N-[2-(dimethylamino)ethyl]-11-phenyl-8-(trifluoromethyl)- 6764-20-1P,
Dibenzo[b,f][1,4]thiazepine-10(11H)-carbonyl chloride 6764-21-2P,
Dibenzo[b,f][1,4]thiazepine-10(11H)-carbonyl chloride, 8-chloro-
6764-23-4P, Dibenzo[b,f][1,4]thiazepine-10(11H)-carboxylic acid,
2-(2-piperidinoethoxy)ethyl ester, oxalate 10493-65-9P,
Dibenzo[b,f][1,4]thiazepine-10(11H)-carboxylic acid, 8-(trifluoromethyl)-,
2-(2-piperidinoethoxy)ethyl ester 10493-66-0P,
Dibenzo[b,f][1,4]thiazepine-10(11H)-carboxylic acid,
2-(dimethylamino)ethyl ester
                              10493-67-1P,
Dibenzo[b,f][1,4]thiazepine-10(11H)-carboxylic acid, 8-chloro-,
2-(dimethylamino)ethyl ester 10493-68-2P,
Dibenzo[b,f][1,4]thiazepine-10(11H)-carboxylic acid, 8-chloro-,
2-(2-piperidinoethoxy)ethyl ester 10510-67-5P.
Dibenzo[b,f][1,4]thiazepine-10(11H)-carboxylic acid,
2-(dimethylamino)ethyl ester, maleate
                                      10510-68-6P.
Dibenzo[b,f][1,4]thiazepine-10(11H)-carboxylic acid, 8-chloro-,
2-(2-piperidinoethoxy)ethyl ester, oxalate 97001-53-1P,
Dibenzo[b,f][1,4]thiazepine-10(11H)-carbonyl chloride, 2,8-dichloro-
97407-65-3P, Dibenzo[b,f][1,4]thiazepine-10(11H)-carbonyl chloride,
11-methvl-
            98655-42-6P, Dibenzo[b,f][1,4]thiazepine,
8-chloro-10,11-dihydro-11-phenyl- 98741-73-2P,
Dibenzo[b,f][1,4]thiazepine-10(11H)-carboxylic acid, 2,8-dichloro-,
2-(dimethylamino)ethyl ester
                              98762-79-9P,
Dibenzo[b,f][1,4]thiazepine-10(11H)-carboxamide,
2.3-dichloro-N-(2-(dimethylamino)ethyl)-
Dibenzo[b,f][1,4]thiazepine-10(11H)-carboxamide,
8-chloro-N-[2-(dimethylamino)ethyl]- 99997-77-0P,
Dibenzo[b, f][1,4]thiazepine-10(11H)-carboxamide,
N-[2-(dimethylamlno)ethyl]-
                             100151-93-7P,
Dibenzo[b,f][1,4]thiazepine-10(11H)-carbonyl chloride, 11-phenyl-
100173-19-1P, Dibenzo[b,f][1,4]thiazepine-10(11H)-carbonyl chloride,
8-chloro-11-phenyl-
                    100356-54-5P,
Dibenzo[b, f][1,4]thiazepine-10(11H)-carboxamide,
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8-chloro-N-[3-(4-methyl-1-piperazinyl)propyl]-, hydrochloride
     100735-21-5P, Dibenzo[b,f][1,4]thiazepine-10(11H)-carboxylic acid,
     8-chloro-, 3-(4-methyl-1-piperazinyl)propyl ester, hydrochloride
     100916-41-4P, Dibenzo[b,f][1,4]thiazepine-10(11H)-carboxamide,
     8-chloro-N-[2-(2-piperidinoethoxy)ethyl]-
                                               101748-62-3P.
     Dibenzo[b, f][1,4]thiazepine-10(11H)-carboxamide,
                                           101957-63-5P,
     N-[2-(diethylamino)ethyl]-11-methyl-
     Dibenzo[b,f][1,4]thiazepine-10(11H)-carboxamide,
     N-|2-(dimethylamino)ethyl|-11-phenyl- 102083-86-3P,
     Dibenzo(b,f)(1,4)thiazepine-10(11H)-carboxamide,
     8-chloro-N-[2-(2-piperidinoethoxy)ethyl]-, oxalate
                                                        102289-22-5P,
     Dibenzo[b,f][1,4]thiazepine-10(11H)-carboxylic acid, 8-chloro-11-phenyl-,
     2-(dimethylamino)ethyl ester
                                   103283-38-1P,
     Dibenzo[b,f][1,4]thiazepine-10(11H)-carboxylic acid, 11-phenyl-,
     2-(dimethylamino)ethyl ester 106302-02-7P,
     Dibenzo[b, f][1,4]thiazepine-10(11H)-carboxamide,
     8-chloro-N-[2-(dimethylamino)ethyl]-11-phenyl-
                                                     106480-71-1P.
     Dibenzo[b,f][1,4]thiazepine, 2,8-dichloro-10,11-dihydro- 106629-93-0P,
     Dibenzo[b,f][1,4]thiazepine-10(11H)-carboxylic acid, 11-methyl-,
     2-(diethylamino)ethyl ester
     RL: PREP (Preparation)
        (preparation of)
     494-20-2P, Dibenzo(b,f)[1,4]thiazepine, 10,11-dihydro-
     RL: PREP (Preparation)
        (preparation of, derivs.)
     ANSWER 48 OF 55 CAPLUS COPYRIGHT 2009 ACS on STN
     1960:100747 CAPLUS
AN
DN
     54:100747
OREF 54:19089f-h
ED
     Entered STN: 22 Apr 2001
ΤI
     Rapid paper ionophoresis using organic buffers in water-formamide aud
     water-urea
AU
    Werum, L. N.; Gordon, H. T.; Thornburg, W.
CS
    Univ. of California, Berkeley
SO
    Journal of Chromatography (1960), 3, 125-45
    CODEN: JOCRAM; ISSN: 0021-9673
DT
    Journal
LA
    English
CC
     2 (General and Physical Chemistry)
     The following organic buffers, in 30% formamide, were used for rapid paper
     ionophoresis in a micro apparatus (buffer and pH given); formate
     -pyridine 3.3, 2-(dimethylamino)ethanol (I)-HCO2H 4.0,
     I-AcOH 4.7, 2,2'-iminodipropionitrile-AcOH 6.0,
     2-(dimethylamino)propionitrile-AcOH 7.2, N-ethylmorpholine-8.0, I-AcOH-H2O
     9.3, I-H3BO3 9.3. As many as 5 different buffers were used
     simultaneously. Charged substances moved as compact spots, without
     adsorption on paper, and with constant mobility in 1-3 hrs. Mobilities were
     measured relative to a set of com. reference dyes, consisting of Amaranth,
     Apollon, Brilliant Blue FCF, and quinacrine-HCl. From mobility values it
     was sometimes possible to estimate the mol. weight, pK value of some acidic or
     basic groups, and the presence of borate-complexing groups. The procedure
    can be applied to the separation and characterization of amino acids, peptides,
     carbohydrates, and proteins (if formamide is replaced by 10% urea).
    Amaranth (the dye)
        (as reference dye in paper ionophoresis)
     Amino acids
     Peptides
     Proteins
        (electrophoresis of)
   Carbohydrates
       (electrophoresis of, on paper)
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Electrophoresis, Electrochromatography
        (with buffers (organic))
     Morpholine, 4-ethyl-, mixture with HOAc
        (as buffer in paper ionophoresis)
     Apolon
        (as reference dye in paper ionophoresis)
     Glycine, N-alanyl-
        (electrophoresis (paper) of)
     100-74-3 915-67-3 926-77-2 1999-33-3
        (Derived from data in the 6th Collective Formula Index (1957-1961))
     69-05-6, Quinacrine, hydrochloride 3844-45-9, Brilliant Blue FCF
        (as reference dye in paper ionophoresis)
     2869-25-2, Propionitrile, 2,2'-iminodi- 5350-67-4, Propionitrile,
     2-dimethylamino-
        (buffer from HOAc and, in paper ionophoresis)
     10043-35-3, Boric acid
        (buffer solution from 2-dimethylaminoethanol and, in paper
        ionophoresis)
     64-19-7, Acetic acid
        (buffer systems, in paper ionophoresis)
     56-12-2, Butyric acid, 4-amino- 107-95-9, β-Alanine 556-33-2, Glycine, N-(N-glycylglycyl)- 556-50-3, Glycine, N-glycyl- 3695-73-6,
     Alanine, N-glycyl- 32729-21-8, Asparagine, glycyl-
        (electrophoresis (paper) of)
     50-99-7, D-Glucose 56-40-6, Glycine 56-41-7, Alanine 56-45-1, Serine
     56-84-8, Aspartic acid 56-86-0, Glutamic acid 57-50-1, Sucrose
     63-42-3, Lactose 71-00-1, Histidine 74-79-3, Arginine 147-85-3,
     Proline 407-41-0, Serine, phosphate 407-41-0, Serine, phosphate
     3458-28-4, Mannose 7664-38-2, Phosphoric acid
        (electrophoresis of)
ΙT
     64-18-6, Formic acid
        (mixts. of, with 2-dimethylaminoethanol and with pyridine, as
        buffers in paper ionophoresis)
     110-86-1, Pyridine
        (mixts. of, with HCO2H, as buffer in paper ionophoresis)
     108-01-0, Ethanol, 2-dimethylamino-
        (mixts. with HOAc, H3BO3 and HCO2H, as buffers in paper ionophoresis)
IT
     1071-23-4, Ethanol, 2-amino-, phosphate
        (paper electrophoresis of)
1.9
    ANSWER 49 OF 55 CAPLUS COPYRIGHT 2009 ACS on STN
AN 1959:112026 CAPLUS
DN 53:112026
OREF 53:20137h-i,20138a-b
ED Entered STN: 22 Apr 2001
TI Sterol aminoalkyl carbonates
IN Bergstrom, Clarence G.
PA G.D. Searle and Co.
DT
   Patent
LA
    Unavailable
    10J (Organic Chemistry: Steroids)
FAN.CNT 1
     PATENT NO.
                        KIND
                                DATE
                                      APPLICATION NO. DATE
                                19590602 US 1957-640990
PI US 2889318
CLASS
 PATENT NO. CLASS PATENT FAMILY CLASSIFICATION CODES
 US 2889318
               IPCR C07D0211-00 [I,C*]; C07D0211-08 [I,A]; C07J0041-00
                       [I,A]; C07J0041-00 [I,C*]; C07J0075-00 [I,A];
                       C07J0075-00 [I,C*]
                 NCL
                       540/113.000; 552/544.000
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AB
    A method is given for the preparation of the title compds., which are useful as
     depressants of the central nervous system. Over 45 min. excess COC12 is
     introduced into a stirred solution of cholesterol 260 in Et20 1850 parts, the
     solution kept at room temperature 18 hrs., a stream of N conducted through the
     solution an addnl. 2 hrs., the solution distilled to dryness in vacuo, and the
     residue recrystd. from Me2CO, to yield 5-cholesten-3β-yl
     chloroformate (I), m. 122-3.5°. I 20 in Me2CO 160 is refluxed, 2-
     dimethylaminoethanol 4 added gradually, the mixture refrigerated,
     the precipitate filtered off and recrystd. from either CHC12-petr. ether or
     Me2CO-CHCl3 to vield 5-cholesten-3β-vl dimethylaminoethyl
     carbonate-HCl (II.HCl), m. 206-8°. II.HCl 10 in CHCl3 750 is
     treated with saturated aqueous NaHCO3 250 with stirring, the CHCl3 washed with
     H2O, dried, MeI 55 parts added, the mixture allowed to stand 4 days,
     filtered, and the residue recrystd. to give II.MeI, m. 204-8°. II
     in Et20 treated with HBr in iso-PrOH gives II.HBr. Prepared similarly, are:
     5-cholesten-3β-yl diethylaminoethyl carbonate-HCl, m. 179-83°,
     and the 5-cholesten-3β-corresponding methiodide, m. 193-5°,
     5-cholesten-3β-yl 3-diethylaminopropyl carbonate-HCl, m.
     186-9°, 5-cholesten-3β-yl dibutylaminoethyl carbonate-HCl, m.
     184-7°, 5-cholesten-3β-yl 3-dibutylaminopropyl carbonate-HCl,
     m. 183-8°, 5-cholesten-3β-yl morpholinoethyl carbonate-HCl, m.
     210-24°, 5-cholesten-3β-yl 2,6-dimethylpiperidinoethyl
     carbonate-HCl, 5-cholesten-3β-yl 2-pyridylmethyl carbonate,
     24-ethyl-5-cholesten-3β-yl chloroformate,
     24-ethyl-5-cholesten-3β-yl dimethylaminoethyl carbonate-HCl, m.
     217-20° (decomposition), and 24-ethyl-5,22-cholestadien-3β-yl
     dimethyl-aminoethyl carbonate-HCl.
    Sterols
        (aminoalkyl carbonates)
    Alcohols
        (aminoalkyl, sterol carbonates)
     Nervous system
        (blocking agents or depressants for central, sterol aminoalkyl
        carbonates as)
     7144-08-3 119599-25-6 119621-82-8
                                              119640-73-2
                                                            120024-35-3
     120037-07-2
                  121144-27-2 121159-34-0
        (Derived from data in the 6th Collective Formula Index (1957-1961))
     57-88-5, Cholesterol
        (aminoalkyl carbonates, and derivs.)
     806646-09-3, B-Sitosterol, carbonate, 2-dimethylaminoethyl ester
        (and derivs.)
     220858-97-9, Ethanol, 2-dimethylamino-, carbonate
        (ester with cholesterol and derivs.)
     463-79-6, Carbonic acid
        (esters, with aminoalkyl alcs. and sterols)
     463-73-0, Formic acid, chloro-
        (esters, with cholesterol derivs.)
     463-73-0P, Formic acid, chloro-, esters, with cholesterol
     120036-59-1P, 1-Propanol, 3-dibutylamino-, carbonate, cholesteryl ester, hydrochloride 121159-29-3P, 1-Propanol, 3-diethylamino-, carbonate,
     cholesteryl ester, hydrochloride
                                        121193-57-5P, Stigmasterol, carbonate,
                                                807297-20-7P, Ammonium,
     2-dimethylaminoethyl ester, hydrochloride
     diethyl(2-hydroxyethyl)methyl-, carbonate, cholesteryl ester
     885459-83-6P, 4-Morpholineethanol, carbonate, cholesteryl ester,
     hydrochloride 896442-03-8P, Ethanol, 2-dibutylamino-, carbonate,
     cholesteryl ester, hydrochloride 896442-10-7P, Ethanol, 2-diethylamino-,
     carbonate, cholesteryl ester, hydrochloride 909265-30-1P, Choline,
     iodide carbonate, cholesteryl ester
     RL: PREP (Preparation)
        (preparation of)
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     ANSWER 50 OF 55 CAPLUS COPYRIGHT 2009 ACS on STN
     1956:79053 CAPLUS
AN
DN
     50:79053
OREF 50:14978c-d
ED
    Entered STN: 22 Apr 2001
     Isolation of radioformaldehyde in the metabolism of
TI
     dimethylaminoethanol-C14H3
ΑU
     Johnston, John M.; Mackenzie, Cosmo G.
CS
    Univ. of Colorado School of Med., Denver
SO
     Journal of Biological Chemistry (1956), 221, 301-5
     CODEN: JBCHA3: ISSN: 0021-9258
DT
     Journal
LA
     Unavailable
CC
     11H (Biological Chemistry: Pharmacology)
    cf. C.A. 48, 8289d. Dimethylaminoethanol-C14H3 (I) was
     synthesized from monomethylaminoethanol, HCO2H, and C14H2O. The specific
     activity of the product indicates that in this reaction CH2O, and not
     formate, is the sole source of the Me C atom. When I was
     incubated with a whole-liver homogenate, C14H2O accumulated and was
     isolated as the dimedon derivative Addition of semicarbazide to the incubation
     mixture increased the yield of C14H2O 3-fold. The implications of these
     results are discussed with respect to the pathway of
     dimethylaminoethanol metabolism
     Metabolism, animal
        (of dimethylaminoethanol)
     14762-75-5P, Carbon, isotope of mass 14
     RL: PREP (Preparation)
        (as indicator, of HCHO formation from dimethylaminoethanol in
        liver preparation)
     108-01-0P, Ethanol, 2-dimethylamino-
     RL: PREP (Preparation)
        (formaldehyde formation from, in liver homogenates)
     9003-33-2P, Poly(divinyl formal)
     RL: PREP (Preparation)
        (formation of, from dimethylaminoethanol by liver homogenate)
     371173-16-9P, Ethanol, 2-(methylmethyl-C14-amino)-
     RL: PREP (Preparation)
        (preparation of)
T.9
     ANSWER 51 OF 55 CAPLUS COPYRIGHT 2009 ACS on STN
AN
     1955:49727 CAPLUS
DN
     49:49727
OREF 49:9705d-a
ED
     Entered STN: 22 Apr 2001
     Conversion of N-methylglycines to active formaldehyde and serine
ΤI
AU
     MacKenzie, Cosmo G.
CS
     Univ. of Colorado School of Med., Denver
SO
     Symposium on Amino Acid Metabolism (Proceedings) (1955) 684-726
     CODEN: 11YDAL
DT
     Journal
LA
     Unavailable
CC
     11A (Biological Chemistry: General)
     Washed rat-liver mitochondria catalyzed the oxidative demethylation of
     dimethylglycine to HCHO and sarcosine. Sarcosine, in turn, was oxidized
     to glycine and HCHO. In both the reactions, the active formaldehyde (AF)
     was the immediate product which could irreversibly convert to HCHO.
     Alternatively, AF could condense with glycine to yield L-serine. The
     nature of AF is not known but it is not identical with aminolevulinic acid
     of Shemin (cf. C.A. 48, 2145h) or the tetrafolic acid derivative of Sakami.
     Expts. with CD3NHCH2COOH (100 atom % excess of D) showed that AF possessed
     an oxidative level of HCHO. No similar oxidative demethylation could
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happen to monomethylaminoethanol, dimethylaminoethanol, choline,

betaine, methylamine, or dimethylamine. Methoxyacetic and methylthioglycolic acids were found to be potent competitive inhibitors in the oxidation. The formation of AF in washed liver mitochondria did not require addition of exogenous coenzymes, such as diphosphopyridine nucleotide or adenine flavine dinucleotide. D-Alanine, but not L-alanine or pyruvate, reduced the serine synthesis but increased O consumption from sarcosine. No HC14HO was isolated when methyl-labeled methionine was incubated with liver slices or mitochondria. M. suggested that biologically labile methyl groups circulated via AF as well as by other processes (transmethylation) without passing through HCHO or formate. Mitochondria (chondriomes, chondriosomes) (dimethylglycine conversion to active formaldehyde and sarcosine in liver) Methyl group (labile, active HCHO and) 107-97-1, Sarcosine (dimethylglycine conversion to, in liver mitochondria) 42854-62-6, Alanine, D-, benzyl ester, p-toluenesulfonate (effect on dimethylglycine conversion to serine in liver mitochondria) 625-45-6, Acetic acid, methoxy-(effect on oxidative demethylation of dimethylalycine in liver mitochondria) 1118-68-9P, Glycine, N,N-dimethyl-RL: PREP (Preparation) (formation of active formaldehyde and sarcosine from, in liver mitochondria) 56-40-6P, Glycine RL: PREP (Preparation) (formation of, from sarcosine in liver mitochondria) 9003-33-2P, Poly(divinyl formal) RL: PREP (Preparation) (formation of, from N,N-dimethylglycine in mitochondria of liver) 56-45-1P, Serine RL: PREP (Preparation) (formation of, from N-methyl glycine in mitochondria of liver) 118685-91-9, Sarcosine-methyl-d3 (in active HCHO expts.) 64-19-7, Acetic acid (sarcosine oxidation inhibition by) ANSWER 52 OF 55 CAPLUS COPYRIGHT 2009 ACS on STN 1955:12687 CAPLUS 49:12687 OREF 49:2573g-i Entered STN: 22 Apr 2001 The role of vitamin B6 and the biosynthesis of choline in the excised tomato root Boll, Wm. Geo. Univ. of Texas, Austin Archives of Biochemistry and Biophysics (1954), 53, 20-8 CODEN: ABBIA4; ISSN: 0003-9861 Journal Unavailable 11D (Biological Chemistry: Botany) cf. C.A. 49, 446i. The following substances replace pyridoxine to a greater or lesser degree in the nutrition of a clone of excised tomato roots: DL-valine, L-valine, DL-norvaline, L-serine, DL-norleucine, DL-cystathionine, L-methionine, L-isoleucine, L-lysine, L-phenylalanine, DL-leucine, L-leucine, DL-α-aminobutyric acid, ethanolamine, dimethylaminoethanol, choline, glycolic acid, and formate

. Ethanolamine does not act as a precursor of vitamin B6. The data

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support the view that choline is formed in the excised tomato root by methylation of ethanolamine; that ethanolamine is formed on decarboxylation of serine by an enzyme containing a component of vitamin B6; that norvaline is involved in normal metabolism; and that vitamin B6 is involved, directly or indirectly, in the biosynthesis of other substances listed above. Tomatoes (choline formation in excised roots of, vitamin B6 in) 56-45-1, Serine 56-87-1, Lysine 56-88-2, Cystathionine 63-68-3, Methionine 63-91-2, Alanine, phenyl- 64-18-6, Formate 72-18-4, Valine 73-32-5, Isoleucine 79-14-1, Glycolic acid 141-43-5, Ethanol, 2-amino- 327-57-1, Norleucine 2835-81-6, Butyric acid, 2-amino-(as vitamin B6 substitute for tomato roots) 61-90-5, Leucine (as vitamin B6 substitute for tomato roots, other) 108-01-0, Ethanol, 2-dimethylamino- 6600-40-4, Norvaline (as vitamin B6 substitute in tomato roots) 62-49-7P, Choline RL: PREP (Preparation) (formation of, in tomato roots, vitamin B6 in) 8059-24-3P, Vitamin, B6 RL: PREP (Preparation) (in choline formation in tomato roots) ANSWER 53 OF 55 CAPLUS COPYRIGHT 2009 ACS on STN 1951:30162 CAPLUS AN 45:30162 OREF 45:5255a-c ED Entered STN: 22 Apr 2001 Biosynthesis of choline methyl groups by the rat Arnstein, H. R. V. ΑU CS Natl. Inst. Med. Research, Mill Hill, London SO Biochemical Journal (1951), 48, 27-32 CODEN: BIJOAK; ISSN: 0264-6021 Journal LA Unavailable CC 11E (Biological Chemistry: Nutrition) AB Addition of choline or betaine to a methionine-free diet enables white rats to use homocystine as the sole S-containing amino acid for growth. Both choline and methionine act as donors of labile CH3 groups, and only betaine and dimethylthetin can replace them. On the contrary, dimethylaminoethanol, though it is a precursor of choline and prevents fatty livers or hemorrhagic kidneys in rats, is not available for growth, presumably because the CH3 groups are not labile. The in vivo synthesis of choline is not sufficiently rapid to supply CH3 groups for optimum growth. The biosynthesis was investigated by feeding D- and L-(β-C14)-serine, (α-C14)-glycine, (C1400H)-glycine, (C14)-methanol, or (C14)-formate to adult rats. The L-serine is converted to ethanolamine by loss of the COOH group, but D-serine does not function as a precursor of choline. MeOH, formate, β-C of L-serine or the α -C (not the carboxyl) of glycine are all precursors of choline CH3 groups. But neither the CO2 arising from in vivo oxidation of D-(β -C14)-serine or from (C1400H)-glycine are such precursors. Methyl group (of choline) 56-45-1, Serine 64-18-6, Formate 67-56-1, Methanol (as choline precursor) 14762-75-5P, Carbon, isotope of mass 14 RL: PREP (Preparation) (as indicator, of choline methyl group formation) 56-40-6P, Glycine

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RL: PREP (Preparation)
        (choline formation from)
     62-49-7, Choline
        (methyl group of, origin of)
     ANSWER 54 OF 55 CAPLUS COPYRIGHT 2009 ACS on STN
L9
AN 1951:19509 CAPLUS
DN
    45:19509
OREF 45:34661,3467a-c
ED
    Entered STN: 22 Apr 2001
TI
    Synthesis of labile methyl groups by the rat
AU
    Sakami, Warwick; Welch, Arnold D.
CS
     Western Reserve Univ., Cleveland, O.
SO
     Journal of Biological Chemistry (1950), 187, 379-84
     CODEN: JBCHA3; ISSN: 0021-9258
DT
     Journal
LA
     Unavailable
     11E (Biological Chemistry: Nutrition)
     Five days prior to, and during, the experiment 100 g. rats were fed asynthetic
     amino acid diet rich in methionine (1.25%) and containing no glycine, serine,
     cystine, choline, or ethanolamine. They were given subcutaneous
     injections of 0.2 ml. 0.15 M C14-labeled Na formate (9.6 +
     106 counts per min. per millimole) at the beginning of the first hr., and
     0.15 ml. for each of 10 succeeding hrs. The animals were then sacrificed,
     and the abdominal viscera were homogenized with acetone, extracted with
     Et20-Et0H, trichloroacetic acid, acetone, and dried. The dry protein was
     demethylated with boiling HI, and the MeI formed was converted into
     tetramethylammonium iodide (I) with trimethylamine. The activity of I
     corresponded to 354 counts per min. per mg. methionine methyl C.
     Formation of labile methyl groups was also found in expts. with rat liver
     slices (6 g.) incubated for 4 hrs. in a medium containing labeled
     formate (8.8 + 106 counts/min.), and nonisotopic
     homocysteine, dimethylaminoethanol, folic acid, and crystalline
     vitamin B12. Methionine and choline were each isolated and converted to
     I. The isotopic activity of I corresponded to 540 counts per min. per mg.
     methionine methyl C, and 530 counts per min. per mg. choline methyl C.
     Folic acid may be involved in the metabolism of 1-carbon compds., such as
     formic acid.
     Methyl group
        (formation of labile)
     Metabolism, animal
        (of carbon (C1) compds., folic acid in)
     Nutrition, animal
        (survey of)
     14762-75-5P, Carbon, isotope of mass 14
     RL: PREP (Preparation)
        (as indicator, of labile Me group formation)
     63-68-3, Methionine
        (carbon-14 in, after administration of labeled HCOONa)
     62-49-7P, Choline
     RL: PREP (Preparation)
        (formation of, from Na formate)
     59-30-3, Folic acid
        (in metabolism of 1-carbon compds.)
     141-53-7P, Sodium formate
     RL: PREP (Preparation)
        (in methyl group (labile) synthesis in animal organism)
1.9
     ANSWER 55 OF 55 CAPLUS COPYRIGHT 2009 ACS on STN
    1947:25565 CAPLUS
AN
DN
    41:25565
OREF 41:5095h-i,5096a-h
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Entered STN: 22 Apr 2001
     Influence of chemical constitution upon toxicity. I. Compounds related to
     "dorvl"
AII
     Haworth, Robert D.; Lamberton, Alex. H.; Woodcock, David
CS
    Univ. Sheffield, UK
SO
    Journal of the Chemical Society (1947) 176-82
     CODEN: JCSOA9; ISSN: 0368-1769
    Journal
LA
    Unavailable
CC
    10 (Organic Chemistry)
    In a study of the influence of chemical constitution upon toxicity, the
AB
     quaternary NH4 salt group was selected for preliminary investigation
     partly on account of the solubility of these compds. in H2O and partly in view
     of the physiol. activity of various derivs. of choline. The high toxicity
     of doryl, H2NCO2(CH2)2NMe3Cl, was confirmed but a wide range of homologs
     and analogs was found to exhibit lower toxicity. C1(CH2)20COC1 (I), b.
     152°, results from 12 g. HO(CH2)2Cl and COCl2 on standing in a
     sealed tube 70 h. at 15°; other chloroformates: 4-chlorobuty1, b10
     89°; 5-chloropentyl, b15 125-30°; 6-chlorohexyl, b12
     120°; 8-chlorooctyl, b12 130°; 9-chlorononyl, b15
     137°; 10-chlorodecvl, b12 170°. I (6.5 g.), gradually
     treated (shaking and cooling) with 15 cc. 15% NH4OH, gives 4.6 g.
     Cl(CH2)20CONH2, m. 76°. In other cases 2.1 mol of the amine in 5
     vols. C6H6 is added to 1 mol of the chloroformate in 5 vols. C6H6 and,
     after 1 h., the filtrate from the amine-HCl is washed with dilute HCl and
     the product distilled or crystallized 2-Iodopropyl carbamate (?) (by
refluxing 12
     h. the Cl derivative and NaI in EtOH), m. 74-6°. 2-Chloroethyl
     alkylcarbamates: Pr, b10 138°; allyl, b10 130°; benzyl, m.
     48°; di-Me, b16 92°; di-Et, b13 100°; di-Pr, b20
     135°; pentamethylene, C5H10NCO2CH2CH2Cl, b17 135°; dibenzyl,
     m. 64°. 2-Iodoethyl bensylcarbamate, m. 92°. Chloroalkyl
     carbamates: 3-chloropropyl, m. 58°; 4-chlorobutyl, m. 74°;
     5-chloroamyl, m. 78°; 6-chlorohexyl, m. 70°; 8-chlorooctyl,
     m. 83°; 9-chlorononyl, m. 77°; 10-chlorodecyl, m.
     84°. Doryl (a type of the quaternary NH4 salts) can be prepared from
     10 cc. Me3n and 6 g. H2NCO2CH2CH2Cl on heating 16 h. at 110-20°;
     careful temperature control is often necessary and anhydrous solvents should be
     used for crystallization The chloride with NaI in cold absolute EtOH gives the
     iodide. The reactions of H2NCO2CH2CH2Cl and the Pr homolog with Et3N,
     Pr3N, and Am3N were studied at temps. from 15° to 180°, both
     in the absence and presence of solvents (ether, C6H6, and PhCH2OH) but
     gave only the HCl salts of the amines. In the following, the m.p. and
     L.D.50 (mg./kg.) are given. Derivs. of trimethyl(2-hydroxyethyl)ammonium
     chloride: urethane (doryl), 207°, 3; N-methylurethane, 173°,
     15; N-ethylurethane, 196-200°, 60; N-propylurethane, 203-7°
     15; N-allylurethane, 167-73°, 37.5; N-phenylurethane, 192°,
     37.5; N,N-dipropylurethane, m. 99°, 75. Derivs. of
     trimethyl(2-hydroxyethyl)ammonium iodide: urethane, 193°, 4.5;
     N-benzylurethane, m. 96°, 62.5; N,N-dimethylurethane, 202°
     20; N, N-diethylurethane, m. 114°, 42.5; 1-piperidylformate,
     178°, 18.5; vinyl ether, 177°, 33; N-methylthiourethane,
     237° (decomposition), 40; N,N-dibenzylurethane, 119-21°,
     75°. Trimethyl(3-hydroxypropyl)ammonium chloride urethane,
     207-9°, 37.5; 4-hydroxybutyl homolog, 212-13°, 12.5;
     5-hydroxyamyl homolog, 195-7°, 22; 6-hydroxyhexyl homolog,
     211-12°, 100; 8-hydroxyoctyl homolog, 205°, 200;
     9-hydroxynonyl homolog, 199°, 185; 10-hydroxydecyl homolog,
     202°, 75. Triethyl(2-hydroxyethyl)ammonium iodide urethane, m. 205°, 395; N-phenylurethane, 128°, 450. I (4 g.) and 3.5 g.
     Me2NNH2 in 50 cc. C6H6, reacting in the cold for 15 min., Me2NNH2.HCl
     removed, and the residue from the C6H6 heated in a sealed tube 5 h. at
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110-20°, give 2-keto-4,4-dimethyl-2,3,5,6-tetrahydro-1,3,4-
oxadiazinium chloride, m. 184°, 194.
4-(2-Hydroxyethyl)morpholine-MeCl urethane, m. 138°, 194. 2-
Dimethylaminoethanol urethane-HCl, m. 144-7°, 1000-2000;
N-methylthiourethane-HCl, m. 97°, 100. Me
2-dimethylaminoethanesulfonate-HCl, m. 97°, 100. Doryl has L.D.50
of 3 mg./kg. for mice and 0.25, mg./kg. for cats and dogs; it has a
constrictor action on the pupil of a cat but this property was not found
with the homologs. Replacement of 1 or both of the amide H atoms by alkyl
groups and an increase in the number of CH2 groups diminish toxicity. There
is some alteration in toxicity with increasing chain length but higher
homologs are definitely less toxic than lower members. Replacement of the
NH2 groups in compds. of the doryl type by hydrazide or ether radicals
results in substances of low toxicity. The high toxicity in the doryl
series depends upon the presence of both urethane and quaternary NH4
groupings.
Toxicity
   (chemical constitution and)
Morpholinium compounds, 4-(2-hydroxyethyl)-4-methyl-, chloride carbamate
RL: PREP (Preparation)
Carbamic acid, dibenzyl-
   (esters)
           2114-18-3P 20074-88-8P 20485-86-3P 20485-87-4P
627-11-2P
114947-88-5P 412308-23-7P 1087717-99-4P
RL: SPN (Synthetic preparation); PRP (Properties); PREP (Preparation)
   (Influence of chemical constitution upon toxicity. I. Compounds related
   to "dorvl")
59-99-4, Neostigmine
   (compds. related to)
107-07-3, Ethanol, 2-chloro- 108-01-0, Ethanol, 2-dimethylamino-
463-73-0, Formic acid, chloro- 928-51-8, 1-Butanol, 4-chloro-
2009-83-8, 1-Hexanol, 6-chloro- 5259-98-3, 1-Pentanol, 5-chloro-
5957-17-5, Ammonium, triethyl(2-hydroxyethyl)-, iodide
Carbamic acid, dimethyl- 13406-98-9, 1-Piperidinecarboxylic acid
23144-52-7, 1-Octanol, 8-chloro- 24579-70-2, Carbamic acid, diethyl-
36887-74-8, Carbamic acid, methylthiono- 50853-31-1, Carbamic acid,
       51308-99-7, 1-Nonanol, 9-chloro- 51309-10-5, 1-Decanol,
10-chloro- 66384-75-6, Carbamic acid, propyl- 69777-50-0, Carbamic
acid, dipropyl-
                85600-10-8, Carbamic acid, benzyl-
   (esters)
62-49-7, Choline
   (esters, and related compds.)
674-38-4P, Bethanechol
RL: PREP (Preparation)
   (preparation and toxicity of)
98-04-4P, Ammonium, trimethylphenyl-, iodide 6140-15-4P, Ammonium,
trimethyl-p-tolyl-, iodides 6326-12-1P, 1-Propanol, 3-chloro-, carbamate
6414-57-9P, Carbamic acid, methyl-, esters with choline chloride
7409-13-4P, Carbamic acid, ethyl-, esters, with choline chloride
24586-04-7P, Ammonium, trimethyl(2-vinyloxyethyl)-, iodide 33046-97-8P,
Ammonium, trimethyl-m-tolyl-, iodides 63867-32-3P, 2H-1,3,4-Oxadiazinium
compounds, tetrahydro-4,4-dimethyl-2-oxo-, chloride 63981-62-4P,
Ammonium, (10-hydroxydecyl)trimethyl-, chloride, carbamate
Ammonium, (4-hydroxybutyl)trimethyl-, chloride, carbamate
                                                          64046-02-2P.
Ammonium, (5-hydroxypentyl)trimethyl-, chloride, carbamate
                                                           856376-66-4P.
Ethanol, 2-iodo-, benzylcarbamate 857169-16-5P, Ammonium,
(6-hydroxyhexyl)trimethyl-, chloride, carbamate 857233-59-1P,
1-Propanol, 3-iodo-, carbamate
                               858824-43-8P, Ammonium,
(8-hydroxyoctyl)trimethyl-, chloride, carbamate 858824-52-9P, Ammonium,
(9-hydroxynonyl)trimethyl-, chloride, carbamate 860707-75-1P, Taurine,
N, N-dimethyl-, methyl ester, hydrochloride
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ΙT

RL: PREP (Preparation)

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(preparation of)
    621-77-2, Tripentylamine
        (reaction with 2-haloethyl carbamate)
     121-44-8. Triethvlamine
        (reactions of, with haloethyl carbamate)
     102-69-2, Tripropylamine
        (reactions with 2-haloethyl carbamate)
=> d his
     (FILE 'HOME' ENTERED AT 12:57:44 ON 19 MAR 2009)
     FILE 'REGISTRY' ENTERED AT 12:58:22 ON 19 MAR 2009
                E N, N-DIMETHYLETHANOLAMMONIUM FORMATE/CN
                E E2
T. 1
              1 S E3
     FILE 'CAPLUS' ENTERED AT 13:01:52 ON 19 MAR 2009
L2
              1 S US20070185330/PN
1.3
              2 S DIMETHYLETHANOLAMMONIUM AND FORMATE
     FILE 'CAPLUS' ENTERED AT 13:15:01 ON 19 MAR 2009
     FILE 'REGISTRY' ENTERED AT 13:15:11 ON 19 MAR 2009
L 4
              2 S 59101-30-3/RN OR 53518-18-6/RN
     FILE 'CAPLUS' ENTERED AT 13:16:40 ON 19 MAR 2009
                S 59101-30-3/REG#
    FILE 'REGISTRY' ENTERED AT 13:18:46 ON 19 MAR 2009
L5
              1 S 59101-30-3/RN
     FILE 'CAPLUS' ENTERED AT 13:18:47 ON 19 MAR 2009
L6
              6 S L5
L7
             56 S (DIMETHYLAMINOETHANOL OR DIMETHYLAMINO ETHANOL) AND (FORMIC O
L8
             0 S IONIC AND L7
L9
             55 S L7 NOT L6
=> s (dimethylaminoethanol or dimethylamino ethanol) and ionic
          2798 DIMETHYLAMINOETHANOL
         77799 DIMETHYLAMINO
        324073 ETHANOL
          1061 DIMETHYLAMINO ETHANOL
                 (DIMETHYLAMINO(W)ETHANOL)
        304581 TONTO
1.10
            62 (DIMETHYLAMINOETHANOL OR DIMETHYLAMINO ETHANOL) AND IONIC
=> s (dimethylaminoethanol or dimethylamino ethanol) and (ionic liquid#)
          2798 DIMETHYLAMINOETHANOL
         77799 DIMETHYLAMINO
        324073 ETHANOL
          1061 DIMETHYLAMINO ETHANOL
                 (DIMETHYLAMINO(W)ETHANOL)
        304581 IONIC
        980632 LIOUID#
         13902 IONIC LIQUID#
                 (IONIC(W)LIQUID#)
             6 (DIMETHYLAMINOETHANOL OR DIMETHYLAMINO ETHANOL) AND (IONIC LIQUI
               D#)
```

=> d 1-6 all

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L11 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2009 ACS on STN
    2007:1252115 CAPLUS
AN
DN
     148 - 223050
ED
     Entered STN: 05 Nov 2007
     Solvent extraction of U(VI) by task specific ionic
     liquids bearing phosphoryl groups
AU
     Ouadi, Ali; Klimchuk, Olga; Gaillard, Clotilde; Billard, Isabelle
CS
     Institut Pluridisciplinaire Hubert Curien, DRS, ULP, CNRS, IN2P3,
     Strasbourg, 67037, Fr.
     Green Chemistry (2007), 9(11), 1160-1162
     CODEN: GRCHFJ; ISSN: 1463-9262
PB
     Royal Society of Chemistry
DT
     Journal
LA
    English
CC
    68-2 (Phase Equilibriums, Chemical Equilibriums, and Solutions)
OS
    CASREACT 148:223050
AB
     A novel class of hydrophobic ionic ligs. based on quaternary ammonium
     cation and bearing phosphoryl groups was synthesized. The preliminary
     results of U(VI) extraction from aqueous solution into the ionic liquid are
presented.
     uranvl extn phosphoryl ammonium ionic lig
     Ouaternary ammonium compounds, properties
     RL: PEP (Physical, engineering or chemical process); PRP (Properties);
     PROC (Process)
        (alkyl; uranyl solvent extraction of U(VI) by task specific ionic ligs.
        bearing phosphoryl groups)
     Ionic liquids
     Partition
     Solvent extraction
        (uranyl solvent extraction of U(VI) by task specific ionic liqs. bearing
        phosphoryl groups)
                                  258273-75-5
     16637-16-4, Uranyl ion(2+)
     RL: PEP (Physical, engineering or chemical process); PRP (Properties);
     PROC (Process)
        (uranyl solvent extraction of U(VI) by task specific ionic liqs. bearing
        phosphoryl groups)
     1005000-61-2P
                   1005000-62-3P
     RL: PEP (Physical, engineering or chemical process); PRP (Properties); SPN
     (Synthetic preparation); PREP (Preparation); PROC (Process)
        (uranyl solvent extraction of U(VI) by task specific ionic liqs. bearing
        phosphoryl groups)
     108-01-0, 2-(Dimethylamino)ethanol
                                          109-55-7.
     3-(Dimethylamino)-1-propylamine
                                      682-76-8, Dibutyl vinylphosphonate
     819-43-2, Dibutyl chlorophosphate
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (uranyl solvent extraction of U(VI) by task specific ionic ligs, bearing
        phosphoryl groups)
     1013924-26-9P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (uranyl solvent extraction of U(VI) by task specific ionic ligs. bearing
        phosphoryl groups)
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```

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- (12) Giridhar, P; J Radioanal Nucl Chem 2005, V265, P31 CAPLUS
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- AN 2006:681182 CAPLUS
- DN 145:145001
- ED
- Entered STN: 14 Jul 2006
- ΤI Preparation of quaternary ammonium compounds as base stable ionic
- Earle, Martyn John; Frohlich, Ute; Hug, Susanne; Katdare, Suhas; Lukasik, IN Rafal Marcin; Bogel, Ewa; Plechkova, Natalia Vladimirovna; Seddon, Kenneth Richard
- The Queen's University of Belfast, UK
- PCT Int. Appl., 35 pp. SO CODEN: PIXXD2
- Patent DT
- LA English
- IC ICM B01J
- CC 21-2 (General Organic Chemistry)

FAN.CNT 1

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EP 1841533

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O.S. MARPAT 145:145001

AB The present invention relates to novel base stable ionic ligs, such as N-alkyl-N,N-dimethylethanolamine salts, N-alkyl-DABCO salts, N-alkyl-tetramethylenediamine salts, and N-alkyl-N-methylpyrazolium salts and uses thereof as solvents in chemical reactions, especially base catalyzed

chemical reactions and reactions comprising the use of strong bases. Chemical reactions include Mannich reaction, Robinson annulation, Michael reaction, Heck reaction, epoxidn., hydrogenation, aldol condensation,

transesterification, esterification, hydrolysis, oxidation, reduction,

hydration.

dehydration, substitution, aromatic substitution, addition (including to carbonyl groups), elimination, polymerization, depolymn., oligomerization, dimerization, coupling, electrocyclisation, isomerization, carbene formation, epimerization, inversion, rearrangement, photochem., microwave assisted, thermal, sonochem. and disproportionation reactions. Thus, N-alkylation of 2-(dimethylamino)ethanol by Pr iodide and treatment of the resulting N-(2-hydroxyethyl)-N, N-dimethyl-Npropylammonium iodide with LiNTf2 (Tf = CF3SO2) gave PrMe2N+CH2CH2OH. [NTf2]-. Cyclopentanone was condensed with pentanal in the presence of L-propine catalyst in EtMe2N+CH2CH2OH.[NTf2]- at room temperature for 18 h to give 94% 2-penty1-2-cyclopenten-1-one.

aldol condensation quaternary ammonium compd solvent prepn; quaternary ammonium compd prepn solvent base stable ionic liq; Mannich reaction Robinson annulation Michael reaction solvent ionic liq; alkyldimethylethanolamine salt prepn solvent base stable ionic liq; alkyl DABCO salt prepn solvent base stable ionic liq; alkyltetramethylenediamine salt prepn solvent base stable ionic liq; alkylmethylpyrazolium salt prepn

solvent base stable ionic liq

Arylation

(Heck; preparation of quaternary ammonium compds. as base stable ionic ligs. as solvents in base-catalyzed chemical reactions)

Cvclization

(Robinson annulation; preparation of quaternary ammonium compds. as base stable ionic ligs. as solvents in base-catalyzed chemical reactions)

Substitution reaction

(aromatic; preparation of quaternary ammonium compds. as base stable ionic ligs. as solvents in base-catalyzed chemical reactions)

Cvclization

(electrocyclic; preparation of quaternary ammonium compds. as base stable ionic ligs, as solvents in base-catalyzed chemical reactions)

Carbenes (methylene derivatives)

RL: SPN (Synthetic preparation); PREP (Preparation)

(formation; preparation of quaternary ammonium compds. as base stable ionic ligs. as solvents in base-catalyzed chemical reactions)

Substitution reaction, nucleophilic

(inversion reaction; preparation of quaternary ammonium compds. as base stable ionic ligs. as solvents in base-catalyzed chemical reactions)

(microwave assisted reactions; preparation of quaternary ammonium compds. as base stable ionic ligs, as solvents in base-catalyzed chemical reactions)

Polymerization

(oligomerization; preparation of quaternary ammonium compds. as base stable ionic ligs. as solvents in base-catalyzed chemical reactions)

Solvents

(organic; preparation of quaternary ammonium compds. as base stable ionic

ligs.

as solvents in base-catalyzed chemical reactions)

Addition reaction

Aldol condensation

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Dehydration reaction
Depolymerization
Dimerization
Disproportionation
Elimination reaction
Epoxidation
Hydration, chemical
Hydrogenation
Hydrolysis
  Ionic liquids
Isomerization
Mannich reaction
Michael reaction
Photolysis
Polymerization
Rearrangement
Reduction
Substitution reaction
Transesterification
   (preparation of quaternary ammonium compds, as base stable ionic ligs, as
   solvents in base-catalyzed chemical reactions)
Quaternary ammonium compounds, preparation
RL: NUU (Other use, unclassified); SPN (Synthetic preparation); PREP
(Preparation); USES (Uses)
   (preparation of quaternary ammonium compds. as base stable ionic ligs. as
   solvents in base-catalyzed chemical reactions)
Reaction
   (sonochem. reactions; preparation of quaternary ammonium compds. as base
   stable ionic ligs. as solvents in base-catalyzed chemical reactions)
Reaction
   (thermal; preparation of quaternary ammonium compds. as base stable ionic
   liqs. as solvents in base-catalyzed chemical reactions)
78-59-1 123-42-2
                    141-79-7 504-20-1
                                          27203-92-5
RL: PRPH (Prophetic)
   (Preparation of quaternary ammonium compounds as base stable
   ionic liquids)
111-66-0P, 1-Octene
                     111-67-1P, 2-Octene
                                           898256-56-9P,
1,3,5-Trimethylpyrazole hydrobromide
RL: BYP (Byproduct); PREP (Preparation)
   (preparation of quaternary ammonium compds. as base stable ionic liqs. as
   solvents in base-catalyzed chemical reactions)
123-75-1, Pyrrolidine, uses 147-85-3, L-Proline, uses
                                                         1305-62-0.
Calcium hydroxide, uses 1310-73-2, Sodium hydroxide, uses 4111-54-0,
Lithium diisopropylamide 6552-73-4, Sodium methoxide-d3 7789-23-3D,
Potassium fluoride, supported on alumina 14014-06-3, Sodium hydroxide-d
20734-58-1, Proton sponge
RL: CAT (Catalyst use); USES (Uses)
   (preparation of quaternary ammonium compds. as base stable ionic liqs. as
   solvents in base-catalyzed chemical reactions)
898256-55-8P
RL: NUU (Other use, unclassified); RCT (Reactant); SPN (Synthetic
preparation); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
   (preparation of quaternary ammonium compds. as base stable ionic liqs. as
   solvents in base-catalyzed chemical reactions)
4535-70-0P, N-Ethyl-N-(2-hydroxyethyl)-N, N-dimethylammonium bromide
7009-61-2P, N-Dodecyl-N-(2-hydroxyethyl)-N, N-dimethylammonium bromide
```

13186-62-4P, N-(2-Hydroxyethyl)-N,N-dimethyl-N-propylammonium bromide 15061-91-3P, N-(2-Hydroxyethyl)-N,N-dimethyl-N-octadecylammonium bromide 28228-54-8P, N-(2-Hydroxyethyl)-N-hexyl-N,N-dimethylammonium chloride 28508-15-8P, N-Butyl-N-(2-hydroxyethyl)-N,N-dimethylammonium bromide

Autoxidation Coupling reaction

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N-Decvl-N-[2-(dimethylamino)ethyl]-N.N-dimethylammonium bromide
171874-92-3P
              202256-55-1P 202256-57-3P 214349-74-3P 219787-58-3P.
N-Hexyl-N-(2-hydroxyethyl)-N, N-dimethylammonium bromide 342789-81-5P
783354-56-3P 852509-35-4P 854102-71-9P 863031-17-8P 885456-22-4P
898256-40-1P 898256-41-2P, N-(2-Butoxvethv1)-N-octv1-N,N-
dimethylammonium bromide 898256-42-3P.
N-12-(Hexvloxy)ethvll-N-hexvl-N, N-dimethvlammonium bromide 898256-43-4P,
N-(2-Butoxyethyl)-N-butyl-N, N-dimethylammonium bromide 898256-44-5P,
N, N-Dimethyl-N-octyl-N-[2-(octyloxy)ethyl]ammonium bromide 898256-45-6P,
N-Decyl-N-[2-(decyloxy)ethyl]-N, N-dimethylammonium bromide 898256-46-7P,
N-Ethyl-N-(2-hydroxyethyl)-N, N-dimethylammonium tetrafluoroborate
898256-47-8P, N-Ethyl-N-(2-hydroxyethyl)-N, N-dimethylammonium
trifluoromethanesulfonate 898256-48-9P,
N-(2-Hydroxyethyl)-N, N-dimethyl-N-propylammonium tetrafluoroborate
898256-49-0P, N-(2-Hydroxyethyl)-N, N-dimethyl-N-propylammonium
trifluoromethanesulfonate 898256-50-3P 898256-51-4P 898256-52-5P
898256-53-6P, N-[2-(Dimethylamino)ethyl]-N,N-dimethyl-N-pentylammonium
bromide 898256-54-7P, N-[2-(Dimethylamino)ethyl]-N,N-dimethyl-N-
                       898256-57-0P 898256-59-2P 898256-60-5P
octvlammonium bromide
898256-61-6P 898256-62-7P 898256-63-8P 898256-66-1P 898256-68-3P 898256-70-7P 898256-75-2P 898256-76-3P 898256-77-4P
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(Preparation); USES (Uses)
   (preparation of quaternary ammonium compds. as base stable ionic liqs. as
   solvents in base-catalyzed chemical reactions)
1128-08-1P, Dihydrojasmone
RL: PNU (Preparation, unclassified); PREP (Preparation)
   (preparation of quaternary ammonium compds. as base stable ionic liqs. as
   solvents in base-catalyzed chemical reactions)
64-17-5, Ethanol, reactions 71-23-8, n-Propanol, reactions 71-36-3,
n-Butanol, reactions 71-41-0, n-Pentanol, reactions 74-96-4, Ethyl
          78-94-4, Methyl vinyl ketone, reactions 106-94-5, n-Propyl
bromide
         107-08-4, Propyl iodide 108-01-0, 2-(Dimethylamino)
ethanol 108-94-1, Cyclohexanone, reactions 109-65-9, n-Butyl
bromide 110-18-9, N.N.N', N'-Tetramethylethylenediamine 110-53-2,
Pentyl bromide 110-62-3, Pentanal 110-91-8, Morpholine, reactions
111-25-1, n-Hexyl bromide 111-27-3, n-Hexanol, reactions 111-83-1, n-Octyl bromide 111-87-5, n-Octanol, reactions 112-29-8, n-Decyl
bromide 112-30-1, 1-Decanol 112-53-8, 1-Dodecanol 112-71-0,
n-Tetradecvl bromide 112-72-1, n-Tetradecanol 112-82-3, n-Hexadecvl
bromide 112-89-0, n-Octadecvl bromide 112-92-5, n-Octadecanol
120-92-3, Cyclopentanone 124-63-0, Methanesulfonyl chloride 143-15-7,
n-Dodecyl bromide 280-57-9, DABCO 504-02-9, 1,3-Cyclohexanedione
544-10-5, n-Hexyl chloride 930-36-9
                                       1072-91-9, 1,3,5-Trimethylpyrazole
1122-58-3, 4-Dimethylaminopyridine 1193-55-1,
2-Methylcyclohexane-1,3-dione 16940-81-1, Hexafluorophosphoric acid
21324-39-0, Sodium hexafluorophosphate 30525-89-4, Paraformaldehyde
36653-82-4, n-Hexadecanol 90076-65-6, Lithium
bis(trifluoromethanesulfonimide)
RL: RCT (Reactant); RACT (Reactant or reagent)
   (preparation of quaternary ammonium compds. as base stable ionic liqs. as
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62-50-0P, Ethyl methanesulfonate 1912-31-8P, Propyl methanesulfonate
1912-32-9P, Butyl methanesulfonate 3240-94-6P, 2-(Morpholin-4-yl)ethyl
chloride 5073-65-4P, 2-Methyl-2-(3-oxobutyl)cyclohexane-1,3-dione
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33249-14-8P 39995-55-6P, N-Decyl-N-(2-hydroxyethyl)-N,N-dimethylammonium bromide 50938-57-3P 62634-05-3P 62634-13-3P 62634-16-6P 62634-17-7P 122135-71-1P, N-(2-Hydroxyethyl)-N,N-dimethyl-N-

octvlammonium bromide 123714-89-6P,

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6222-16-8P, Tetradecyl methanesulfonate 6968-20-3P, Pentyl
     methanesulfonate 16156-50-6P, Hexyl methanesulfonate
                                                               16156-52-8P,
     Octvl methanesulfonate 16424-35-4P, 2-Pentylidenecyclopentanone
     20779-14-0P, Hexadecvl methanesulfonate
                                               26942-62-1P,
     2-(3-0xobutv1)cvclohexanone 32492-73-2P.
     N-(2-Hydroxyethyl)-N, N-dimethyl-N-propylammonium iodide 34084-81-6P,
     2-(3-0xobutyl)cyclohexane-1,3-dione 41233-29-8P, Decyl methanesulfonate
     42558-01-0P, 2-(1-Hydroxypentyl)cyclopentanone 159438-86-5P, Undecyl
     methanesulfonate
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        (preparation of quaternary ammonium compds. as base stable ionic liqs. as
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     100-58-3, Phenylmagnesium bromide
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        (preparation of quaternary ammonium compds. as base stable ionic liqs. as
        solvents in base-catalyzed chemical reactions)
     1196-55-0P, 2,3,4,4a,5,6,7,8-Octahydronaphthalen-2-one
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     2-[(Morpholin-4-y1)methy1]cyclohexanone 25564-22-1P,
     2-Pentyl-2-cyclopenten-1-one 42576-97-6P,
     1,2,3,4,6,7,8,8a-Octahydronaphthalene-1,6-dione 99178-63-9P,
     4-[2-[2-(Dimethylamino)ethoxy]ethyl]morpholine
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    Preparation of quaternary ammonium compounds as basic ionic
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                                                                 20070822
PRAI GB 2005-29
                        A
                              20050104
    WO 2006-GB6
                        W
                              20060104
CLASS
PATENT NO.
               CLASS PATENT FAMILY CLASSIFICATION CODES
WO 2006072775
                TCM
                       B01.T
                IPCI
                       B01J0031-02 [I,C]; B01J0031-02 [I,A]; C07B0037-00
                       [I,C]; C07B0037-04 [I,A]; C07C0045-00 [I,C];
                       C07C0045-62 [I,A]; C07C0045-69 [I,A]; C07C0045-72
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                       C07C0045-73 [I,A]; C07C0045-74 [I,A]; C07C0209-00
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                       C07D0233-00 [I,C*]; C07D0233-54 [I,A]; C07D0301-00
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                       C07C217/08; B01J031/02B; B01J031/02C; B01J031/02E;
                       B01J031/02E4; B01J031/02G; B01J031/02G2; C07B061/00;
                       C07C045/51B2+47/228; C07C045/62+47/228;
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                       C07C045/72+49/497; C07C045/72+49/707;
                       C07C045/73+49/403; C07C045/74+49/203;
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                       C07D233/54C: C07D303/32: L01J: L01J: L01J: L01J: L01J:
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EP 1853385
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                       C07B0037-00 [I.C*]
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                       C07C045/51B2+47/228; C07C045/62+47/228;
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                        C07C045/73+49/403; C07C045/74+49/203;
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                        C07D233/54C; C07D303/32; L01J; L01J; L01J; L01J; L01J;
                        L01J; L01J; L01J; M07D
JP 2008526821
               IPCI
                       C07C0211-62 [I,A]; C07C0211-00 [I,C*]; C07C0309-04
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                        [I,A]; C07C0255-00 [I,C*]; C07C0253-30 [I,A];
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                        C07B0061-00 [N,A]
                 FTERM 4C048/AA01; 4C048/BB15; 4C048/CC01; 4C048/UU03;
                        4C048/XX02; 4C048/XX05; 4C055/AA04; 4C055/BA01;
                        4C055/CA01; 4C055/DA52; 4C055/DB02; 4C055/FA01;
                        4C055/FA37; 4C064/AA06; 4C064/CC02; 4C064/DD01;
                        4C064/EE01; 4C064/FF03; 4C064/GG01; 4C064/HH04;
                        4C069/AA02; 4C069/BB02; 4C069/BB16; 4C069/BB34;
                        4C069/CC13; 4H006/AA01; 4H006/AA03; 4H006/AB40;
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                        4H006/BJ50; 4H006/BN20; 4H006/BP10; 4H006/BP30;
                        4H006/BR70; 4H006/BU50; 4H039/CA19; 4H039/CA40;
                        4H039/CA41; 4H039/CA42; 4H039/CE90; 4H039/CF30;
                        4H039/CH10; 4H039/CH20
KR 2007104899 IPCI
                       B01J0031-02 [I,A]; B01J0031-00 [I,A]; B01D0011-04 [I,A]
 CN 101137437
                IPCI
                       B01J0031-02 [I,A]; C07D0301-12 [I,A]; C07D0301-00
                       [I,C*1; C07C0209-60 [I,A]; C07C0209-00 [I,C*];
                       C07C0045-72 [I,A]; C07C0045-69 [I,A]; C07C0045-62
                        [I,A]; C07C0045-00 [I,C*]; C07B0037-04 [I,A];
                        C07B0037-00 [I,C*]
os
    CASREACT 145:145000; MARPAT 145:145000
AB
     This invention relates to preparation and use of ionic ligs, as solvents in
     base-catalyzed chemical reactions wherein the ionic liquid is composed of at
     least one species of cation and at least one species of anion,
     characterized in that a cation of the ionic liquid comprises a pos. charge
     moiety and a basic moiety, and further wherein such ionic ligs. may be
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C07C217/08: B01J031/02B: B01J031/02C: B01J031/02E:

ECLA

reactions, epoxidn., hydrogenation, condensation, oxidation reduction, hydration, dehydration, substitution, aromatic substitution, addition (including to carbonyl groups), elimination, polymerization, depolymn., oligomerization, dimerization, coupling, electrocyclic, isomerization, carbene formation, epimerization, inversion, rearrangement, photochem., microwave assisted,

include Heck Reaction, Suzuki coupling, nucleophilic displacement reactions, hydrolysis, esterification, transesterification, aldol

used as promoters or catalysts for the chemical reactions. Chemical reactions

```
thermal, sonochem. and disproportionation reactions. Thus, etherification
of 2-(dimethylamino)ethanol with
2-(diisopropylamino)ethanol hydrochloride followed by regioselective
quaternization with Et bromide and treatment with lithium bis(triflimide)
gave a room temperature ionic liquid of formula
PrNMe2N+CH2CH2OCH2CH2N(i-Pr)2.N-(SO2CF3)2 (I). Epoxidn. of chalcone in
this ionic liquid I gave chalcone epoxide with 100% conversion.
quaternary ammonium compd prepn solvent catalyst ionic liq
Arvlation
   (Heck; preparation of quaternary ammonium compds. as basic ionic ligs. in
   base-catalyzed chemical reactions)
Substitution reaction
   (aromatic; preparation of quaternary ammonium compds. as basic ionic ligs.
   base-catalyzed chemical reactions)
Cvclization
   (electrocyclic; preparation of quaternary ammonium compds. as basic ionic
   ligs. in base-catalyzed chemical reactions)
Carbenes (methylene derivatives)
RL: SPN (Synthetic preparation); PREP (Preparation)
   (formation; preparation of quaternary ammonium compds. as basic ionic ligs.
   in base-catalyzed chemical reactions)
Reaction
   (inversion; preparation of quaternary ammonium compds. as basic ionic ligs.
   in base-catalyzed chemical reactions)
Reaction
   (microwave-assisted; preparation of quaternary ammonium compds. as basic
   ionic ligs. in base-catalyzed chemical reactions)
Polymerization
   (oligomerization; preparation of quaternary ammonium compds. as basic ionic
   ligs. in base-catalyzed chemical reactions)
Addition reaction
Aldol condensation
Condensation reaction
Coupling reaction
Dehydration reaction
Depolymerization
Dimerization
Disproportionation
Elimination reaction
Epimerization
Epoxidation
Hydration, chemical
Hydrogenation
Hydrolysis
  Ionic liquids
Isomerization
Oxidation
Photolysis
Polymerization
Rearrangement
Reduction
Substitution reaction
Substitution reaction, nucleophilic
Suzuki coupling reaction
Transesterification
   (preparation of quaternary ammonium compds. as basic ionic liqs. in
   base-catalyzed chemical reactions)
Quaternary ammonium compounds, uses
RL: CAT (Catalyst use); NUU (Other use, unclassified); USES (Uses)
   (preparation of quaternary ammonium compds. as basic ionic liqs. in
   base-catalyzed chemical reactions)
```

IT

in

ΤТ

IT Reaction (sonochem.; preparation of quaternary ammonium compds. as basic ionic ligs.

in base-catalyzed chemical reactions)

IT Reaction (thermal; preparation of quaternary ammonium compds. as basic ionic liqs. in

base-catalyzed chemical reactions) IT 78-59-1 123-42-2 141-79-7 504-20-1 15409-60-6 67382-39-2 123134-25-8

RL: PRPH (Prophetic)

(Preparation of quaternary ammonium compounds as basic ionic liquids)

147-85-3, L-Proline, uses 3375-31-3

RL: CAT (Catalyst use); USES (Uses)

(preparation of quaternary ammonium compds. as basic ionic liqs. in base-catalyzed chemical reactions)

898535-34-7P

RL: CAT (Catalyst use); NUU (Other use, unclassified); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent); USES (USes)

(preparation of quaternary ammonium compds. as basic ionic liqs. in base-catalyzed chemical reactions)

33249-14-8P 50938-57-3P 62634-05-3P 62634-13-3P 62634-16-6P 106303-35-9P 114203-57-5P, 62634-17-7P 4-(Dimethylamino)-1-ethylpyridinium bromide 123714-89-6P 171874-92-3P 171894-19-2P, N-[2-(Dimethylamino)ethyl]-N, N-dimethyl-N-octadecylammonium 202256-55-1P 202256-57-3P 214349-74-3P 289910-39-0P, bromide N-Ethyl-N-[2-(dimethylamino)ethyl]-N, N-dimethylammonium bromide 395677-61-9P, 4-(Dimethylamino)-1-hexylpyridinium bromide 863031-17-8P 898256-51-4P 898256-52-5P 898256-53-6P. N-[2-(Dimethylamino)ethyl]-N.N-dimethyl-N-pentylammonium bromide 898256-54-7P, N-[2-(Dimethylamino)ethyl]-N, N-dimethyl-N-octylammonium 898256-84-3P, 4-(Dimethylamino)-1-ethylpyridinium bromide 898256-85-4P 898535-32-5P 898535-36-9P methanesulfonate 898535-38-1P 898535-40-5P 898535-42-7P 898535-44-9P 898535-44-9P 898535-49-4P 898535-51-8P 898535-53-0P 898535-47-2P RL: CAT (Catalyst use); NUU (Other use, unclassified); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)

(preparation of quaternary ammonium compds. as basic ionic liqs. in base-catalyzed chemical reactions)

62-50-0, Ethyl methanesulfonate 74-96-4, Ethyl bromide 75-03-6, Ethyl 78-94-4, Vinvl methyl ketone, reactions 94-41-7, Chalcone 96-79-7, 2-(Diisopropylamino)ethyl chloride 100-52-7, Benzaldehyde, reactions 105-56-6, Ethyl cyanoacetate 106-94-5, n-Propyl bromide 108-01-0, N,N-Dimethylethanolamine 109-65-9, n-Butyl bromide 110-18-9. N,N,N',N'-Tetramethylethylenediamine 110-53-2, n-Pentyl bromide 110-62-3, Pentanal 111-18-2 111-25-1, n-Hexvl bromide 111-83-1, n-Octvl bromide 112-29-8, n-Decvl bromide 112-71-0, n-Tetradecvl bromide 112-82-3, n-Hexadecyl bromide 112-89-0, n-Octadecyl bromide 120-92-3, Cyclopentanone 120-94-5, 1-Methylpyrrolidine n-Dodecyl bromide 280-57-9, DABCO 504-02-9, 1,3-Cyclohexanedione 513-42-8, 2-Methyl-2-propenol 542-69-8, n-Butyl iodide 598-56-1, N-Ethyldimethylamine 616-47-7, 1-Methyl-1H-imidazole 1122-58-3, 1193-55-1, 2-Methylcyclohexane-1,3-dione 4-Dimethylaminopyridine 1704-62-7, 2-[2-(Dimethylamino)ethoxy]ethanol 3647-69-6, 1-(Morpholin-4-yl)-2-chloroethane hydrochloride 4261-68-1, 2-(Diisopropylamino)ethyl chloride hydrochloride 5073-65-4, 2-Methyl-2-(3-oxobutyl)cyclohexane-1,3-dione 13586-68-0 16156-50-6, Hexyl methanesulfonate 35779-04-5, 4-tert-Butyl-1-iodobenzene 90076-65-6, Lithium bis(trifluoromethanesulfonimide) RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of quaternary ammonium compds. as basic ionic liqs. in base-catalyzed chemical reactions)

```
16424-35-4P, 2-Pentylidenecyclopentanone
                                              25564-22-1P.
     2-Penty1-2-cyclopenten-1-one 34084-81-6P,
     2-(3-0xobutv1)cvclohexane-1,3-dione
                                           42558-01-0P,
     2-(1-Hydroxypentyl)cyclopentanone 99178-63-9P,
     4-[2-[2-(Dimethylamino)ethoxy]ethyl]morpholine
                                                      898535-33-6P.
     N, N-Diisopropyl-N-[2-[2-(dimethylamino)ethoxy]ethyl]amine
                                                                898535-45-0P
     959467-54-0P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (preparation of quaternary ammonium compds, as basic ionic ligs, in
        base-catalyzed chemical reactions)
     80-54-6P, β-Lilial 2169-69-9P, Ethyl
     (E)-2-benzylidene-2-cyanoacetate 5411-12-1P, Chalcone epoxide
     14533-87-0P, Ethyl (Z)-2-benzylidene-2-cyanoacetate
                                                          42576-97-6P
     100348-93-4P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (preparation of quaternary ammonium compds. as basic ionic liqs. in
        base-catalyzed chemical reactions)
RE.CNT 5
             THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE
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(2) Anon; US 20020035297 A1 CAPLUS
(3) Anon; US 20040097755 A1 CAPLUS
(4) Anon: WO 2004029004 A1 CAPLUS
(5) Anon: WO 2005019185 A1 CAPLUS
I.11 ANSWER 4 OF 6 CAPLUS COPYRIGHT 2009 ACS on STN
     2005:561949 CAPLUS
AN
DN
     143:229956
ED
    Entered STN: 30 Jun 2005
TΙ
     Synthesis and Characterization of Organometallic Ionic
     Liquids and a Heterometallic Carbene Complex Containing the
     Chromium Tricarbonyl Fragment
AU
    Moret, Marc-Etienne; Chaplin, Adrian B.; Lawrence, Adrien K.; Scopelliti,
     Rosario; Dyson, Paul J.
CS
     Institut des Sciences et Ingenierie Chimiques, EPFL-BCH, Lausanne,
     CH-1015, Switz.
SO
     Organometallics (2005), 24(16), 4039-4048
     CODEN: ORGND7; ISSN: 0276-7333
PR
    American Chemical Society
DT
    Journal
LA
    English
CC
    29-11 (Organometallic and Organometalloidal Compounds)
     Section cross-reference(s): 75
os
     CASREACT 143:229956
AB
     Direct reaction between [Cr(CO)6] and arenes with ionic substituents
     affords the corresponding arene-Cr tricarbonvl complexes,
     [Cr(CO)3(arene)], in only modest (4-32%) yield. In contrast, these
     complexes can be prepared in pure form in excellent yield from the reaction
     of [Cr(CO)3(n6-C6H5CH2Br)] with, for example, N-methylimidazole. The
     structures of [Cr(CO)3(\eta6-C6H5CH2MIM)]Br(MIM = 3-methylimidazolium),
     [Cr(CO)3(\eta6-C6H5CH2MMIM)]Br(MMIM = 2,3-dimethylimidazolium), and
     [Cr(CO)3(n6-C6H5CH2NMe2Me2OH)]Br were established by x-ray diffraction
     anal. Subsequent exchange of the bromide anion for Tf2N- affords new
     organometallic salts with m.ps. <70°. Reaction of the bromide
     salts includes tosylation of [Cr(CO)3(η6-C6H5CH2NMe2Me2OH)]Br to
     afford [Cr(CO)3(η6-C6H5CH2NMe2(CH2)2OTs)]Br and the formation of the
     heterometallic carbene complex [Ru(η6-p-cymene)C12{C4H5N2CH2Ph-η6-
    Cr(CO)3}]. Both compds. were characterized in the solid state by x-ray
    diffraction.
   chromium tricarbonyl derivatized ionic liq prepn; benzylimidazolium
    chromium tricarbonyl deriv prepn structure reaction; ruthenium chromium
```

heterometallic carbene benzylimidazole deriv prepn structure; crystal structure chromium tricarbonyl benzylimidazolium heterometallic ruthenium benzylimidazole carbene; mol structure chromium tricarbonyl

benzylimidazolium heterometallic ruthenium benzylimidazole carbene

T Crystal structure

Molecular structure

(of chromium tricarbonyl benzylimidazolium organometallic ionic liqs. and chromium-ruthenium heterometallic benzylimidazole carbene complex)

IT Ionic liquids

(organometallic; preparation and structure of chromium tricarbonyl benzylimidazolium-containing ionic liqs. and of chromium-ruthenium heterometallic benzylimidazole carbene complex)

IT Aromatic hydrocarbons, reactions

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation and structure of chromium tricarbonyl

benzylimidazolium-containing

ionic liqs. and of chromium-ruthenium heterometallic benzylimidazole carbene complex)

IT 862999-66-4P 862999-67-5P 862999-68-6P

RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(crystal structure; preparation and structure of chromium tricarbonyl benzylimidazolium-containing ionic liga, and of chromium-ruthenium heterometallic benzylimidazole carbene complex)

IT 862999-72-2P 862999-74-4P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (crystal structure; preparation and structure of chromium tricarbonyl benzylimidazolium-containing ionic liqs. and of chromium-ruthenium heterometallic benzylimidazole carbene complex)

IT 108-01-0, 2-(Dimethylamino)ethanol 616-47-7,

N-Methylimidazole 637-59-2 1733-94-0, 1,2-Dimethylimidazole 7221-41-2 13007-92-6, Chromium hexacarbonyl 52462-29-0 65039-11-4 191352-83-9 862999-80-2 862999-81-3

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation and structure of chromium tricarbonyl benzylimidazolium-containing

ionic liqs. and of chromium-ruthenium heterometallic benzylimidazole carbene complex)

500996-04-3P 862999-75-5P 862999-76-6P 862999-77-7P 862999-78-8P 862999-79-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and structure of chromium tricarbonyl

benzylimidazolium-containing

ionic liqs. and of chromium-ruthenium heterometallic benzylimidazole carbene complex)

862999-57-3P 862999-59-5P 862999-61-9P 862999-63-1P 862999-65-3P 862999-69-7P 862999-70-0P 862999-71-1P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation and structure of chromium tricarbonyl

benzylimidazolium-containing

ionic liqs. and of chromium-ruthenium heterometallic benzylimidazole carbene complex)

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- L11 ANSWER 5 OF 6 CAPLUS COPYRIGHT 2009 ACS on STN
- AN 2004:753469 CAPLUS
- DN 141.280342
- ED Entered STN: 16 Sep 2004
- TΙ Polymer particle dispersions, electrolytes and quasi-solid electrolytes comprising same dispersions, and batteries employing same quasi-solid electrolytes
- IN Nagano, Toshiaki; Ogawa, Tetsuo
- PA Kansai Paint Co., Ltd., Japan
- SO Jpn. Kokai Tokkyo Koho, 15 pp. CODEN: JKXXAF
- Patient.
- LA Japanese
- ICM C08F002-12 IC
 - ICS C08F012-00; C08F020-00; H01B001-06; H01M008-02; H01M010-40; H01M014-00
- 52-2 (Electrochemical, Radiational, and Thermal Energy Technology) Section cross-reference(s): 38, 76

FAN CNT 1

PATENT NO.				APPLICATION NO.	
	A		JP 2003-50180		
	CLASS		FAMILY CLAS	SIFICATION CODES	
JP 2004256711		C08F00	1M008-02;		
	IPCI	C08F000 [ICS,7] H01M00	02-12 [ICM,7]; H01B0001-]; C08F0012-00 [ICS, 06 [ICS,7]; H01M0008]; H01M0010-36 [ICS,	-02 [ICS,7];
	IPCR	C08F000 [I,A]; C08F000 [N,C*]; H01M000	02-12 [I,A]; C08F0012-00 20-00 [I,C*]; H01M0008-0	C08F0002-12 [I,C*]; [I,C*]; C08F0020-00; H01B0001-06 [N,A]; 2 [N,A]; H01M0008-02; H01M0010-40 [N,A];	[I,A]; H01B0001-06 [N,C*];
	FTERM	4J011/2 4J011/1 5G301/0 5H026/1 5H029/1	AA05; 4J011/ KB19; 4J011/ CA30; 5G301/ HH05; 5H026/ CJ09; 5H029/	KA01; 4J011/KA15; 4J KB28; 4J011/KB29; 4J CD01; 5H026/AA06; 5H HH06; 5H029/AJ06; 5H HJ01; 5H029/HJ05; 5H AS16; 5H032/EE01; 5H	011/KB30; 026/HH01; 029/AM16; 029/HJ20;

AR Polymer particle dispersions comprise ionic liqs. as disperse media. Also claimed are electrolytes with elec. conductivity between (1 + 10-9) and (1

5H032/EE16; 5H032/HH01; 5H032/HH04; 5H032/HH08

- + 107) S/cm. The (quasi-solid) electrolytes are suitable for
- dye-sensitized solar cells, secondary lithium batteries, and fuel cells. polymer particle dispersion ionic liq medium; electrolyte polymer particle
- dispersion ionic liq; quasi solid electrolyte polymer particle dispersion ionic liq; lithium battery quasi solid electrolyte ionic liq disperse medium; dye sensitized battery quasi solid electrolyte ionic liq dispersion
- Secondary batteries
 - (lithium; polymer particle dispersions containing ionic liquid disperse media, for (quasi-solid) electrolytes and batteries)
- Electrolytes
 - Ionic liquids
 - (polymer particle dispersions containing ionic liquid disperse media, for (quasi-solid) electrolytes and batteries)
- ΤТ Solar cells
 - (quasi-solid electrolytes; polymer particle dispersions containing ionic liquid disperse media, for (quasi-solid) electrolytes and batteries)
- Battery electrolytes (quasi-solid; polymer particle dispersions containing ionic liquid disperse
- media, for (quasi-solid) electrolytes and batteries) 64-19-7DP, Acetic acid, reaction products with cresol novolak epoxy resins
- and amines, polymer with acrylic monomers 100-42-5DP, Styrene, polymers with cresol novolak epoxy resins quaternary ammonium salts, polymer with acrylic monomers 108-01-0DP, N.N-Dimethylaminoethanol,
- reaction products with cresol novolak epoxy resins and acetic acid,
 - polymer with acrylic monomers 6606-59-3DP, 1,6-Hexanediol
 - dimethacrylate, polymers with cresol novolak epoxy resins quaternary
 - ammonium salts, polymer with acrylic monomers 78949-77-6P,
 - 1.6-Hexanediol dimethacrylate-styrene copolymer 181140-08-9DP, ESCN 195
 - acrylate, reaction products with amines and acetic acid, polymer with acrylic monomers 757973-29-8P 757973-30-1P 757973-31-2P
 - RL: DEV (Device component use); IMF (Industrial manufacture); TEM
- (Technical or engineered material use); PREP (Preparation); USES (Uses) (crosslinked, particles; polymer particle dispersions containing ionic

liquid

- disperse media, for (quasi-solid) electrolytes and batteries) 35935-34-3, 1-Methyl-3-ethylimidazolium iodide
 - RL: DEV (Device component use); TEM (Technical or engineered material use); USES (Uses)
 - (ionic ligs.; polymer particle dispersions containing ionic liquid disperse media, for (quasi-solid) electrolytes and batteries)
- L11 ANSWER 6 OF 6 CAPLUS COPYRIGHT 2009 ACS on STN
- AN 2004:56092 CAPLUS
- DN 140:270820
- ED Entered STN: 23 Jan 2004
- ΤТ Triazine-Based Polyfluorinated Triquaternary Liquid Salts: Synthesis, Characterization, and Application as Solvents in Rhodium(I)-Catalyzed Hydroformylation of 1-Octene
- ΑU Omotowa, Bamidele A.; Shreeve, Jean'ne M.
- Department of Chemistry, University of Idaho, Moscow, ID, 83844-2343, USA CS
- SO Organometallics (2004), 23(4), 783-791 CODEN: ORGND7; ISSN: 0276-7333
- PB American Chemical Society
- DT Journal
- LA English
- 28-19 (Heterocyclic Compounds (More Than One Hetero Atom)) Section cross-reference(s): 23, 67
- OS CASREACT 140:270820
- Silylation of N-(2-hydroxyethyl)imidazole, HOCH2CH2Im (1), with AB hexamethyldisilazane gave N-(2-trimethylsilyloxyethyl)imidazole, Me3SiOCH2CH2Im (2), which underwent quaternization reactions with the

alkyl halides and gave three new N-(trimethylsilyloxyethyl) imidazolium halides, Me3SiOCH2CH2Im+RX-, where Im+ = imidazolium and R/X = Me/I (3), CH2CH2F/Br (4), and CH2CH2CF3/I (5). The Et ether, formed from 1 and Et bromide was quaternized with CF3CH2CH2I followed by anion exchange with LiN(SO2CF3)2 to obtain [CF3CH2CH2Im+CH2CH2OEt N(SO2CF3)2-] (8). The metathesis reactions of 3-5 with cyanuric fluoride in acetonitrile at 25° gave tris[2-(N'-alkylimidazolium)ethoxy]triazine trihalides, N3C3(OCH2CH2Im+RX-)3, where R/X = Me/I (9), CH2CH2F/Br (10), and CH2CH2CF3/I (11). Two neutral trimeric compds., N3C3(OCH2CH2Im)3 (12) and N3C3(OCH2CH2NMe2)3 (14), were prepared from reactions of cyanuric fluoride and Me3SiOCH2CH2NMe2 or 2, resp. The quaternization of 12 with MeI gave tris[oxoethyl(trimethyl)ammonium]triazine, N3C3(OCH2CH2N+Me3I-)3 (14). Subsequent exchange of the halides in 9-11 and N3C3(OCH2CH2N+Me3I-)3 (15) with the weakly coordinating anions of AgOSO2CF3, LiN(SO2CF3)2, AgNO3, or AgClO4 resulted in new triquaternary salts that were characterized by NMR, elemental analyses, and, for some of the compds., mass spectroscopy. Phys. (m.p. and d.) and thermal properties of compds. prepared were determined with differential scanning calorimeter (DSC) and thermogravimetric analyzer (TGA). In Rh(I)-catalyzed hydroformylation of 1-octene, with Ph2P(NMPBTA) [NMPBTA = N-methylpyridinium bis(trifluoromethanesulfonyl)amide| as ligand, the turnover frequency (TOF), conversion, isomer selectivity (n/i), and recyclability were compared when triguaternary salts or monoguaternary were used as solvents in the biphasic hydroformylation process. A change of metal/ligand ratio resulted in significant increase of n/i selectivity, but was marginal with 8 as solvent.

triazine polyfluorinated triquaternary lig salt prepn solvent; rhodium catalyzed hydroformylation octene polyfluorinated triazine triguaternary liq solvent; thermogravimetric thermal property polyfluorinated triazine triquaternary liq salt solvent

Solvents

(ionic ligs.; synthesis, characterization, and application of triazine-based polyfluorinated triquaternary liquid salts as solvents in rhodium-catalyzed hydroformylation of octene)

Quaternary ammonium compounds, preparation

RL: NUU (Other use, unclassified); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)

(solvents; synthesis, characterization, and application of triazine-based polyfluorinated triquaternary liquid salts as solvents in rhodium-catalyzed hydroformylation of octene)

Differential scanning calorimetry

Hydroformylation catalysts Ionic liquids

Thermal properties

Thermogravimetric analysis

(synthesis, characterization, and application of triazine-based polyfluorinated triguaternary liquid salts as solvents in rhodium-catalyzed hydroformylation of octene)

673686-75-4P 673687-58-6P 673687-65-5P

RL: NUU (Other use, unclassified); PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(solvent, thermal properties; synthesis, characterization, and application of triazine-based polyfluorinated triguaternary liquid salts as solvents in rhodium-catalyzed hydroformylation of octene)

14874-82-9, (Acetylacetonato)dicarbonylrhodium

RL: CAT (Catalyst use); USES (Uses)

(synthesis, characterization, and application of triazine-based polyfluorinated triquaternary liquid salts as solvents in rhodium-catalyzed hydroformylation of octene)

673687-18-8P

RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP

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(Preparation); RACT (Reactant or reagent)
        (synthesis, characterization, and application of triazine-based
       polyfluorinated triquaternary liquid salts as solvents in
       rhodium-catalyzed hydroformylation of octene)
    107-07-3, 2-Chloroethanol, reactions 108-01-0, 2-N,N-
                          111-66-0, 1-Octene 288-32-4, Imidazole,
    Dimethylaminoethanol
    reactions 460-37-7, 3,3,3-Trifluoropropyl iodide 675-14-9, Cyanuric
    fluoride
              762-49-2, 1-Bromo-2-fluoroethane 1079-66-9,
    Chlorodiphenylphosphine 3430-13-5, 5-Bromo-2-methylpyridine
    90076-65-6, Lithium bis(trifluoromethylsulfonyl)amide
    RL: RCT (Reactant); RACT (Reactant or reagent)
        (synthesis, characterization, and application of triazine-based
       polyfluorinated triquaternary liquid salts as solvents in
       rhodium-catalyzed hydroformylation of octene)
    1615-14-1P, 1-(2-Hydroxyethyl)imidazole 16654-64-1P
                                                            132682-77-0P
    197712-86-0P 673686-35-6P 673686-67-4P 673687-75-7P
    RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (synthesis, characterization, and application of triazine-based
       polyfluorinated triquaternary liquid salts as solvents in
       rhodium-catalyzed hydroformylation of octene)
    124-19-6P, Nonanal 7786-29-0P, 2-Methyloctanal
    RL: SPN (Synthetic preparation); PREP (Preparation)
        (synthesis, characterization, and application of triazine-based
       polyfluorinated triquaternary liquid salts as solvents in
       rhodium-catalyzed hydroformylation of octene)
    673687-83-7P
    RL: CAT (Catalyst use); RCT (Reactant); SPN (Synthetic preparation); PREP
     (Preparation); RACT (Reactant or reagent); USES (Uses)
        (thermal properties; synthesis, characterization, and application of
       triazine-based polyfluorinated triquaternary liquid salts as solvents in
       rhodium-catalyzed hydroformylation of octene)
    132684-26-5P 673686-41-4P 673686-48-1P
                                                 673686-55-0P
                                                                 673686-81-2P
    673686-87-8P 673686-90-3P 673686-95-8P
                                                673687-12-2P
                                                                 673687-24-6P
    673687-32-6P 673687-39-3P 673687-46-2P 673687-50-8P
    RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP
     (Preparation); RACT (Reactant or reagent)
        (thermal properties; synthesis, characterization, and application of
       triazine-based polyfluorinated triquaternary liquid salts as solvents in
       rhodium-catalyzed hydroformylation of octene)
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L12 12 "WALKER ADAM J"/AU OR "WALKER ADAM JOHN"/AU
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6 "WALKER ADAM J"/AU 6 "WALKER ADAM JOHN"/AU

=> s e2 or e3

=> d 1-12 all

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L13 ANSWER 1 OF 12 CAPLUS COPYRIGHT 2009 ACS on STN
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AN 2007:619447 CAPLUS

DN 147:33228

ED Entered STN: 08 Jun 2007

TI Use of hydroxylammonium salts as ionic liquid solvents for

enzyme-catalyzed reactions IN Walker, Adam John

PA Bionigs Limited, UK

SO PCT Int. Appl., 38pp.

CODEN: PIXXD2

DT Patent

LA English

CC 45^-5 (Industrial Organic Chemicals, Leather, Fats, and Waxes) Section cross-reference(s): 23

FAN.CNT 1

FAN	.CNT																		
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PI WO 2007063327										WO 2006-GB4503									
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								DE,											
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								LK,											
								NA,											
								SG,					SY,	TJ,	TM,	TN,	TR,	TT,	
		DM.						VC,					EТ	ED	CD	CD	шп	TE	
		KW:						MC,											
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								C07C											
				IPC				-00									11-0	0	
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				IPC	R			-00				239-	10 f	I,Al	; C0	7C00	59-0	0	
								07C0											
						C07C	0311	-00	[I,C]; C	07C0	311-	49 [I,A]	; C1	2P00	01-0	0	
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								7-62											
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OS MARPAT 147:33228

An lonic liquid comprises cations of the formula R1R2R3N+-OR4, where R1, R2, R3 and R4 are each independently selected from hydrogen and hydrocarbyl, the ionic liquid containing < 1% of water. The ionic liquid containing < 1% of water. The ionic liqs. may be used as solvents for chemical or biochem. reactions, in particular, for enzyme-catalyzed reactions. Thus, N,N-diethylhydroxylammonium acetate (m.p. < -20°, viscosity 12 cP

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at 25°, refractive index 1.414) was prepared by dissolving
     N,N-diethylhydroxylamine (90) and acetic acid (60.06 q) sep. in ethanol
     (250 mL each), and adding the acid solution dropwise to the amine solution over
     1 h, while cooling with ice and stirring.
ST
    hydroxylammonium salt ionic lig solvent enzyme catalyzed
     reaction
    Solvents
        (organic; use of hydroxylammonium salts as ionic liquid solvents
        for enzyme-catalyzed reactions)
     Ionic liquids
        (use of hydroxylammonium salts as ionic liquid solvents for
        enzyme-catalyzed reactions)
     Enzymes, uses
     RL: CAT (Catalyst use); USES (Uses)
        (use of hydroxylammonium salts as ionic liquid solvents for
        enzyme-catalyzed reactions)
     Quaternary ammonium compounds, preparation
     RL: IMF (Industrial manufacture); NUU (Other use, unclassified); PREP
     (Preparation); USES (Uses)
        (use of hydroxylammonium salts as ionic liquid solvents for
        enzyme-catalyzed reactions)
     39004-71-2P, N.N-Diethvlhvdroxvlammonium acetate
                                                       939384-89-1P
     939384-90-4P
                   939384-91-5P 939384-93-7P 939384-94-8P 939384-96-0P
     939384-97-1P
     RL: IMF (Industrial manufacture); NUU (Other use, unclassified); PREP
     (Preparation); USES (Uses)
        (use of hydroxylammonium salts as ionic liquid solvents for
        enzyme-catalyzed reactions)
     939384-92-6P
     RL: IMF (Industrial manufacture); NUU (Other use, unclassified); RCT
     (Reactant); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
        (use of hydroxylammonium salts as ionic liquid solvents for
        enzyme-catalyzed reactions)
                                     75-75-2, Methanesulfonic acid
     64-19-7, Acetic acid, reactions
                                                                      79-14-1,
     Glycolic acid, reactions 108-01-0, N,N-Dimethylethanolamine
                                                                   121-44-8,
     Triethylamine, reactions 127-09-3, Sodium acetate 1493-13-6, Triflic
           3710-84-7, N,N-Diethylhydroxylamine 7647-01-0, Hydrochloric acid,
     reactions
                7722-84-1, Hydrogen peroxide, reactions 82113-65-3,
     Bis(trifluoromethylsulfonyl)imide
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (use of hydroxylammonium salts as ionic liquid solvents for
        enzyme-catalyzed reactions)
RE.CNT 19
             THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE
(1) Anon
(2) Anon
(3) Anon
(4) Anon
(5) Anon
(6) Anon
(7) Anon
(8) Anon; GAZZ CHIM ITAL 1954, V84, P915
(9) Anon; J AM CHEM SOC 1927, V49, P1539
(10) Anon; J AM CHEM SOC 1947, V69, P1731
(11) Anon; J CHIN CHEM SOC 1977, V24, P115
(12) Anon; J MOL STRUCT 1990, V239, P1
(13) Anon; JUSTUS LIEBIGS ANN CHEM 1913, V397, P275
(14) Anon; YAKUGAKU ZASSHI 1940, V60, P24
(15) Hecht Stacie E; US 2006094616 Al 2006
(16) Nippon Telegraph & Telephone; JP 2005149982 A 2005 CAPLUS
(17) Takami, N; JP 11086905 A 1999 CAPLUS
(18) Umemoto Teruo; US 2006094882 A1 2006
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- (19) Wehner Wolfgang; US 4578489 A 1986 CAPLUS
- L13 ANSWER 2 OF 12 CAPLUS COPYRIGHT 2009 ACS on STN
- AN 2007:371437 CAPLUS
- DN 146:379587
- ED Entered STN: 04 Apr 2007
- TI Primary, secondary and tertiary ammonium salts as ionic liquids
- IN Walker, Adam John
- PA Bionigs Limited, UK
- SO Brit. UK Pat. Appl., 51pp.
- CODEN: BAXXDU
- DT Patent
- LA English
- CC 23-4 (Aliphatic Compounds)
- FAN.CNT 1

PAN.	CMI	1																
PATENT NO.					KIND DATE				APPLICATION NO.						DATE			
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						MZ,												
						SE,												
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						UZ,												
		RW:				CH,												
			IS,	IT,	LT,	LU,	LV,	MC,	NL,	PL,	PT,	RO,	SE,	SI,	SK,	TR,	BF,	BJ,
			CF.	CG.	CI.	CM,	GA.	GN.	GO.	GW.	ML.	MR.	NE.	SN.	TD.	TG.	BW.	GH.
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			BA,															
	JP	2009	5100	38		T		2009	0312		JP 2	008-	5328	63		2	0060	928
	TN	2008	KN01	698		A		2008	1226		TN 2	008-	KN16	9.8		2		
	IIS	2008 2008	0221	361		7.1		2008	0911		HS 2	008-	8850	a		2	0080 0800	502
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	CIN	1013 2005	1001	0		A		2008 2005	1203		CN Z	006-	0004	4643			0080	529
PRAI	GB	2005	-198	98		A.		2005	0930									
	GB	2006	-191	30		A3		2006	0928									
	WO	2006 2006	-GB3	586		W		2006	0928									
CLAS																		
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						[I,A	1; 0	07C0	215-	00 [I,Cl	; C0	7C02	15-0	8 [I	.A1:		
						C07C	0215	-12	II.A	1: 0	0700	215-	40 f	T.A1	: C0	7002	17-2	8 [I,A]
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						[I,C												
				IPC	R	C07C	0217	-00	[I,C]; (07C0	217-] 80	I,A]	; B0	1J00	31-0	0
						[I,C	*];	B01J	0031	-00	[I, A]; B	01J0	031-	02 [I,C]	;	
						B01J												40
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ECLA
                      C07C215/40; B01J031/00E; B01J031/02G2; C07C217/08;
GB 2444614
                TPCT
                       C07C0215-08 [I,A]; C07C0215-12 [I,A]; C07C0215-40
                       [I,A]; C07C0215-00 [I,C*]; C07C0217-08 [I,A];
                       C07C0217-00 [I.C*]
                IPCR
                       C07C0215-00 [I,C]; C07C0215-08 [I,A]; B01J0031-00
                       [I,C*]; B01J0031-00 [I,A]; B01J0031-02 [I,C*];
                       B01J0031-02 [I,A]; C07C0215-12 [I,A]; C07C0215-40
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                       C07C0217-28 [I.A]
EP 1948589
                IPCI
                       C07C0217-08 | I.A|; C07C0217-28 | I.A|; C07C0217-00
                       [I,C*]; B01J0031-02 [I,A]
JP 2009510038
                IPCI
                       C07C0217-08 [I,A]; C07C0217-00 [I,C*]
                FTERM 4H006/AA01; 4H006/AB81; 4H006/BN10; 4H006/BP10;
                       4H006/BU50
IN 2008KN01698 TPCT
                       C07C0217-08 [ICM, 7]; C07C0217-00 [ICM, 7, C*]
US 20080221361 IPCI
                       C07C0217-08 [I,A]; C07C0217-28 [I,A]; C07C0217-00
                       [I,C*]
                NCL
                       564/508.000; 564/503.000
CN 101316810
                IPCI
                       C07C0217-08 [I,A]; C07C0217-28 [I,A]; C07C0217-00
                       [I,C*]; B01J0031-02 [I,A]
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OS MARPAT 146:379587

- AB The invention provides ionic liqs. and processes for their preparation The liqs. comprise a cation of the formula N+HRIR2R3. Ammonium salts of formula N+HRIR2R3: wherein Rl is (un)substituted hydrocarbyl-oxy-hydrocarbyl; R2 and R3 is H and hydrocarbyl; R2R3 taken together with the N to form a heterocyclic group; are claimed. In each instance hydrocarbyl should be understood as any group containing carbon and hydrogen, which may also contain one or more heteroatoms. Preferred anions include halides, halogenated inorg, or organic anions, nitrates, sulfates, phosphates, carboxylates, sulfonates and carbonates. These ionic ligs. may be useful as solvents for chemical or bio-chemical, particularly enzyme-catalyzed, reactions.
- ST amine carboxylic acid salt formation; ammonium salt prepn ionic lig
- T Ionic liquids

(preparation of primary, secondary and tertiary ammonium salts as ionic ligs.)

IT Quaternary ammonium compounds, preparation

RL: NUU (Other use, unclassified); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); USES (Uses) (preparation of primary, secondary and tertiary ammonium salts as

ionic ligs.)

III 13695-28-8P 13695-29-9P 68052-35-7P 162783-72-4P 205490-68-2P 523978-47-4P 932394-16-6P 932394-10-1P 932394-111-1P 932394-12-2P 932394-13-3P 932394-14-4P 932394-15-5P 932394-16-6P 932394-17-7P 932394-18-8P 932394-19-9P 932394-20-2P 932394-21-3P 932394-22-4P 932394-22-5P 932394-29-5P 932394-25-7P 932394-26-6P 932394-27-9P 932394-28-0P 932394-29-1P 932394-30-4P 932394-31-5P 932394-32-6P

RL: NUU (Other use, unclassified); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)

(preparation of primary, secondary and tertiary ammonium salts as ionic liqs.)

T79-09-4, Propanoic acid, reactions 79-14-1, Glycolic acid, reactions 100-37-8, N,M-Diethylethanolamine 111-75-1, N-Butylethanolamine 124-07-2, Octanoic acid, reactions 621-56-7, 1-(Diethylamino)propan-2,3-diol 1704-62-7,

N, N-Dimethy1-[2-(2-hydroxyethoxy)ethy1]amine 3030-44-2,

N,N-Dimethyl-2-methoxyethylamine 3179-63-3, N,N-Dimethylpropanolamine 5332-73-0, 3-Methoxypropylamine 16369-21-4, N-Propylethanolamine 92260-33-8, N-Methyl-bis-(2-methoxyethyl)amine

RL: RCT (Reactant); RACT (Reactant or reagent) (preparation of primary, secondary and tertiary ammonium salts as ionic ligs.) RE CNT 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD RE (1) Anon: US 20030149264 A CAPLUS (2) Anon; WO 2004114445 A CAPLUS (3) Anon; GB 2412912 A CAPLUS (4) Anon; US 4377654 A CAPLUS L13 ANSWER 3 OF 12 CAPLUS COPYRIGHT 2009 ACS on STN AN 2006:343657 CAPLUS DN 144:390206 ED Entered STN: 14 Apr 2006 ΤТ Use of ionic liquids as media for catalyzed reactions Walker, Adam John; Gimpel, Erik Richard; Rosser, Susan Jane IN Cambridge University Technical Services Limited, UK PA SO PCT Int. Appl., 40 pp. CODEN: PIXXD2 DT Patent English LA IC ICM B01J031-02 ICS B01J019-00 21-3 (General Organic Chemistry) Section cross-reference(s): 7, 9, 63, 67 FAN.CNT 1 KIND DATE APPLICATION NO. PATENT NO. WO 2006038013 A2 20060413 WO 2005-GB3848 W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM GB 2420344 A 20060524 GB 2005-20313 20051006 EP 1804969 A2 20070711 EP 2005-788999 R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, AL, BA, HR, MK, YU T 20080515 JP 2007-535237 JP 2008515619 US 20080191170 A1 20080814 US 2007-576822 20071116 20041008 PRAI GB 2004-22447 A WO 2005-GB3848 W 20051006 CLASS PATENT NO. CLASS PATENT FAMILY CLASSIFICATION CODES WO 2006038013 ICM B01J031-02 ICS B01J019-00 IPCI B01J0031-02 [ICM, 7]; B01J0019-00 [ICS, 7] TPCR B01J0031-00 [I,C*]; B01J0031-00 [I,A]; B01J0031-02 [I,C*]; B01J0031-02 [I,A]; B01J0039-00 [I,C*]; B01J0039-04 [I,A]; B01J0041-00 [I,C*]; B01J0041-04 [I,A]; C07B0061-00 [I,C*]; C07B0061-00 [I,A]; C12N0009-04 [I,C*]; C12N0009-04 [I,A] ECLA B01J039/04; B01J031/00E; B01J031/02G2; B01J031/02G4D;

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B01J041/04; C07B061/00; C12N009/04; L01J
GB 2420344
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                       C07D0233-54 [I,A]; C07D0233-00 [I,C*]; C07C0213-00
                       [I,A]; C07C0213-08 [I,A]; C07C0215-08 [I,A];
                       C07C0215-12 [I,A]; C07C0215-00 [I,C*]; C12P0017-18
                       [I.A]
                 IPCR
                       C07D0233-00 [I,C]; C07D0233-54 [I,A]; B01J0031-00
                       [I,C*]; B01J0031-00 [I,A]; B01J0031-02 [I,C*];
                       B01J0031-02 [I,A]; B01J0039-00 [I,C*]; B01J0039-04
                       [I,A]; B01J0041-00 [I,C*]; B01J0041-04 [I,A];
                        C07B0061-00 [I,C*]; C07B0061-00 [I,A]; C07C0213-00
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                        C07C0215-00 [I,C]; C07C0215-08 [I,A]; C07C0215-12
                        [I,A]; C12N0009-04 [I,C*]; C12N0009-04 [I,A];
                        C12P0017-18 [I,C]; C12P0017-18 [I,A]
                 ECLA
                        B01J039/04; B01J031/00E; B01J031/02G2; B01J031/02G4D;
                        B01J041/04; C07B061/00; C12N009/04; L01J
EP 1804969
                 TPCT
                       B01J0031-02 [I,A]; B01J0019-00 [I,A]
                 IPCR
                       B01J0031-02 [I,C]; B01J0031-02 [I,A]; B01J0019-00
                       [I,C]; B01J0019-00 [I,A]; B01J0031-00 [I,C*];
                        B01J0031-00 [I,A]; B01J0039-00 [I,C*]; B01J0039-04
                        [I,A]; B01J0041-00 [I,C*]; B01J0041-04 [I,A];
                        C07B0061-00 [I,C*]; C07B0061-00 [I,A]; C12N0009-04
                        [I,C*]; C12N0009-04 [I,A]
                 ECLA
                       B01J039/04; B01J031/00E; B01J031/02G2; B01J031/02G4D;
                        B01J041/04; C07B061/00; C12N009/04; L01J
JP 2008515619
                        B01J0019-00 [I,A]; C07C0215-40 [N,A]; C07C0215-00
                 TPCT
                        [N,C*]; C07C0053-08 [N,A]; C07C0053-18 [N,A];
                       C07C0053-00 [N,C*]
                 IPCR
                       B01J0019-00 [I,C]; B01J0019-00 [I,A]; B01J0031-00
                       [I,C*]; B01J0031-00 [I,A]; B01J0031-02 [I,C*];
                        B01J0031-02 [I,A]; B01J0039-00 [I,C*]; B01J0039-04
                        [I,A]; B01J0041-00 [I,C*]; B01J0041-04 [I,A];
                       C07B0061-00 [I,C*]; C07B0061-00 [I,A]; C07C0053-00
                        [N,C]; C07C0053-08 [N,A]; C07C0053-18 [N,A];
                       C07C0215-00 [N,C]; C07C0215-40 [N,A]; C12N0009-04
                        [I,C*]; C12N0009-04 [I,A]
                 FTERM 4G075/AA13; 4G075/BA10; 4G075/BB03; 4G075/CA51;
                        4G075/CA54; 4G075/CA55; 4G075/DA18; 4H006/AA03;
                        4H006/AB99; 4H006/BM10; 4H006/BM71; 4H006/BN10;
                        4H006/BU32
US 20080191170 IPCI
                       B01F0001-00 [I,A]
                 NCL
                       252/364.000
    A method of using an ionic liquid involves in the order specified,
     providing an ionic liquid having a first chemical form, using the
     first chemical form ionic liquid for a first predetd, purpose, chemical
     modifying the first chemical form ionic liquid so as to change it to
     a second chemical form, and using the second chemical ionic liquid for a
     second determined purpose. Thus, 3-hydroxypropylmethylimidazolium
     hexafluorophosphate was converted to the trimethylsilyl compound which could
     be deprotected to back to the hexafluorophosphate compound
    ionic liq carrier medium catalyzed reaction prepn
ΙT
    Bases, uses
     RL: NUU (Other use, unclassified); USES (Uses)
        (Bronsted bases; use of ionic ligs, as media for catalyzed
        reactions)
     Basicity
        (Lewis; use of ionic ligs. as media for catalyzed reactions)
     Solvation
        (affinity; use of ionic liqs. as media for catalyzed
        reactions)
    Heat capacity
        (specific; use of ionic ligs. as media for catalyzed
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reactions)
    Bronsted acidity
     Chirality
     Dielectric constant
     Dissociation constant
     Electric conductivity
     Electric conductors
     Electric insulators
     Electromagnetism
    Electron acceptors
    Electron donors
    Electrophoresis
     Freezing point
     Hydrogen bond
     Interfacial tension
     Ion exchangers
      Ionic liquids
     Lewis acidity
     Melting point
     Polarity
     Reaction kinetics
     Reactivity (chemical)
     Redox potential
     Refractive index
     Sensors
     Solvents
     Thermal conductivity
     Thermal conductors
     Thermal insulators
    Viscosity
        (use of ionic ligs. as media for catalyzed reactions)
    97002-71-6, Morphine dehydrogenase
     RL: BSU (Biological study, unclassified); CAT (Catalyst use); BIOL
     (Biological study); USES (Uses)
        (use of ionic liqs. as media for catalyzed reactions)
     670222-24-9
                 823179-37-9
     RL: NUU (Other use, unclassified); USES (Uses)
        (use of ionic ligs. as media for catalyzed reactions)
     RL: NUU (Other use, unclassified); RCT (Reactant); SPN (Synthetic
     preparation); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
        (use of ionic ligs, as media for catalyzed reactions)
     721942-97-8P
                  866568-18-5P
                                  866569-32-6P
     RL: NUU (Other use, unclassified); SPN (Synthetic preparation); PREP
     (Preparation); USES (Uses)
        (use of ionic ligs. as media for catalyzed reactions)
     69-57-8, Penicillin G sodium
     RL: PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES
     (Uses)
        (use of ionic ligs. as media for catalyzed reactions)
     3724-65-0, Crotonic acid
                              355011-34-6
                                              866568-01-6
                                                           866568-90-3
     866569-40-6
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (use of ionic liqs. as media for catalyzed reactions)
     882848-41-1P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (use of ionic liqs. as media for catalyzed reactions)
L13 ANSWER 4 OF 12 CAPLUS COPYRIGHT 2009 ACS on STN
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AN 2006:247293 CAPLUS

Entered STN: 17 Mar 2006

ED

- Task-specific ionic liquids for biomolecular applications
- Walker, Adam J.; Bruce, Neil C. AU
- CS Bioniqs, York, YO10 5DG, UK
- so Abstracts of Papers, 231st ACS National Meeting, Atlanta, GA, United States, March 26-30, 2006 (2006), IEC-282 Publisher: American Chemical Society, Washington, D. C. CODEN: 69HYEC
- Conference; Meeting Abstract; (computer optical disk)
- LA English
- AB Ionic ligs, have attracted considerable recent attention as "designer solvents", due to the large number of potential low-melting anion/cation combinations and the significant differences in phys. and chemical properties between them. To date, however, most research involving ionic liqs. has utilized a limited range of these compds. originally devised for electrochem. applications and little effort has been made to tailor the solvent design process towards the particular requirements of other industrially relevant processes. Based upon our studies into the interactions between ionic ligs. and biol. mols., we have developed new classes of ionic ligs. specifically optimized as solvents for biochem. processes, including enzyme catalysis, protein stabilization and assay techniques. These materials also offer advantages over conventional ionic ligs. in terms of safety, biodegradability, viscosity and cost.
- L13 ANSWER 5 OF 12 CAPLUS COPYRIGHT 2009 ACS on STN
- 2006:247128 CAPLUS AN
- ED Entered STN: 17 Mar 2006
- TI Redox biocatalysis in ionic liquids
- AU Stubley, Heather C.; Walker, Adam J.; Bruce, Neil C.
- CS Department of Biology, University of York, York, Y010 3LR, UK SO
- Abstracts of Papers, 231st ACS National Meeting, Atlanta, GA, United States, March 26-30, 2006 (2006), IEC-117 Publisher: American Chemical Society, Washington, D. C. CODEN: 69HYEC
- DT Conference; Meeting Abstract; (computer optical disk)
- LA English
- AB Enzymes are remarkable catalysts, ideal for organic synthesis. In vivo enzymic reactions occur in water, but problems arise due to poor substrate solubility and proteolysis. Studying enzymes in non-aqueous systems provides novel
- information about enzyme reactions and allow impossible or marginal reactions to occur. Studies in organic solvents show enzymes can be active in non-aqueous solvents. Ionic ligs, have great potential for enzyme catalysis, they are powerful solvents that are liquid at room temperature
 - and composed only of ions. They lack vapor pressure, are generally polar with varying phys. properties. Their characteristics arise through the asym. interaction of the cation and anion. They can be tailored by altering the ion composition, allowing the solvent to be designed around an enzyme. This study focuses on activity and stability of alc. dehydrogenase (ADH) in ionic ligs., structure of ADH in ionic ligs. and effect of water content upon enzyme structure and activity.
- L13 ANSWER 6 OF 12 CAPLUS COPYRIGHT 2009 ACS on STN
- ΔN 2006:247126 CAPLUS
- ED Entered STN: 17 Mar 2006
- Effects of anion and cation selection on the physical properties of ammonium based ionic liquids
- Gimpel, Erik R.; Walker, Adam J. AII
- CS Research, Bioniqs Ltd, York, Y010 5DG, UK
- SO Abstracts of Papers, 231st ACS National Meeting, Atlanta, GA, United

States, March 26-30, 2006 (2006), IEC-115 Publisher: American Chemical Society, Washington, D. C. CODEN: 69HYEC

- DT Conference; Meeting Abstract; (computer optical disk)
- LA English
- AB Ionic ligs. exhibit numerous interesting properties, notably they are non-volatile, non-flammable and can dissolve extremely high concns. of a wide variety of materials. Conventional ionic ligs., however, suffer from disadvantages such as cost, high viscosity and are often hazardous to both workers and the environment. We present new solvents which are cheap, readily prepared and purified, biodegradable (>98% in 48 h) and exhibit low viscosities (10-50 mPa.s). These solvents may be tailored for specific tasks including targeted solubilisation, purification or removal of particular materials or the performance of enzyme-catalyzed reactions. Selection of the appropriate ions enables the fine tuning of properties, including viscosity and solubility where a single bond alter these values by over an order of magnitude. Significant changes can be achieved by interchanging functional groups; process relevant properties that can be adjusted include lipophilicity, hydrogen bonding, chemical and thermal stability.
- L13 ANSWER 7 OF 12 CAPLUS COPYRIGHT 2009 ACS on STN
- AN 2006:247125 CAPLUS
- ED Entered STN: 17 Mar 2006
- Biocatalysis in novel functionalized ionic liquids
- Falcioni, Francesco; Walker, Adam J.; Bruce, Neil C. AII
- CNAP, Department of Biology, University of York, York, Y010 5DD, UK Abstracts of Papers, 231st ACS National Meeting, Atlanta, GA, United States, March 26-30, 2006 (2006), IEC-114 Publisher: American Chemical Society, Washington, D. C. CODEN: 69HYEC
- DT Conference; Meeting Abstract; (computer optical disk)
- LA English
- AB Ionic liqs. used as biocatalytic solvents can overcome the limitations imposed by water by dissolving higher concns. of organic substrates, while offering major advantages in replacing mol. solvents, owing to their compatibility with high-order biomol. structures, negligible vapor pressure, non-flammability, stability and recyclability. The majority of ionic ligs, studied so far belong to the dialkylimidazolium group and suffer from high viscosity, difficult product recovery, significant toxicity and unproven biodegradability. Rational functionalisation of ionic ligs, can improve their performance: a range of novel ionic ligs, based upon functionalised alkanolammonium nuclei offer significant improvements over imidazolium salts and their analogs,. This project aims to address their application as alternative media for biocatalysis using purified hydrolases. A comparative study of activity and conformation through complementary techniques will clarify the nature of the interactions between protein and ionic liqs. and identify the parameters directing the choice of the best ionic liquid for a given biocatalytic reaction.
- L13 ANSWER 8 OF 12 CAPLUS COPYRIGHT 2009 ACS on STN 2005:1170512 CAPLUS
- AN
- DN 143:435309
- Entered STN: 03 Nov 2005 ED
- Affinity chromatography using ionic liquids TN
- Walker, Adam John PA The University of York, UK
- SO PCT Int. Appl., 23 pp.
- CODEN: PIXXD2 DT Patent
- LA English

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ICM C07K001-22
     ICS C12N011-14
     9-3 (Biochemical Methods)
     Section cross-reference(s): 1, 3, 4, 7, 15, 50
FAN.CNT 1
    PATENT NO.
                       KIND DATE APPLICATION NO. DATE
                       ----
                        A1 20051103 WO 2005-GB1549 20050421
    WO 2005103070
        W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH,
            CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,
             GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ,
             LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA,
             NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL,
             SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA,
             ZM, ZW
         RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM,
             AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK,
             EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT,
             RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML,
            MR, NE, SN, TD, TG
                                           GB 2006-22206
     GB 2429284
                         A
                               20070221
                                                                 20050421
     GB 2429284
                         В
                               20080730
PRAI GB 2004-8854
                         Α
                               20040421
    WO 2005-GB1549
                         W
                               20050421
 PATENT NO. CLASS PATENT FAMILY CLASSIFICATION CODES
WO 2005103070
                ICM
                       C07K001-22
                ICS
                       C12N011-14
                 IPCI
                       C07K0001-22 [ICM, 7]; C07K0001-00 [ICM, 7, C*];
                       C12N0011-14 [ICS, 7]; C12N0011-00 [ICS, 7, C*]
                 IPCR
                       C07K0001-00 [I,C*]; C07K0001-22 [I,A]; C12N0011-00
                       [I,C*]; C12N0011-00 [I,A]; C12N0011-14 [I,A]
                 ECLA
                       C07K001/22; C12N011/00
                       C07K0001-22 [I,A]; C12N0011-14 [I,A]; C07K0001-00
GB 2429284
                 IPCI
                       [I,C]; C07K0001-22 [I,A]; C12N0011-00 [I,C];
                       C12N0011-14 [I,A]
                 IPCR
                       C07K0001-00 [I,C]; C07K0001-22 [I,A]; C12N0011-00
                       [I,C]; C12N0011-00 [I,A]; C12N0011-14 [I,A]
                       C07K001/22; C12N011/00; C12N011/14
   The present invention relates to a composition for separating a target mol.
from, or
     in, an ionic liquid the composition comprising: (iii) a liquid medium
     comprising an ionic liquid; and (ii) a binding agent that is bound
     to a support wherein the binding agent is specific for a target mol.
ST
    affinity chromatog ionic lig
тт
    Bond
        (-disrupting agent; affinity chromatog, using ionic ligs.)
IT
     Functional groups
        (Alkenyl; affinity chromatog, using ionic ligs.)
     Reaction
        (Biol. or chemical; affinity chromatog, using ionic ligs.)
     Proteins
     RL: ANT (Analyte); CPS (Chemical process); NUU (Other use, unclassified);
     PEP (Physical, engineering or chemical process); ANST (Analytical study);
     PROC (Process); USES (Uses)
        (DNA-binding; affinity chromatog, using ionic ligs.)
    Apparatus
        (Filtration; affinity chromatog, using ionic ligs.)
    Anions
       (Halogenated inorg.; affinity chromatog. using ionic liqs.)
     Interface
```

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(Phase; affinity chromatog, using ionic ligs.)
        (Quaternary nitrogen or phosphorus-based; affinity chromatog, using
       ionic lias.)
    Functional groups
        (Thio; affinity chromatog, using ionic ligs.)
    Affinity chromatography
    Amino group
    Anions
    Binders
    Carbonyl group
    Carboxyl group
    Cations
    Chemical formula
    Columns and Towers
    Composition
    Drugs of abuse
    Dyes
    Explosives
    Filaments
    Functional groups
    Hydroxyl group
      Ionic liquids
    Liquid chromatography
    Micelles
    Molecules
    Nanoparticles
    Pharmaceutical analysis
    Separation
    Solids
    Solutions
    Volume
    Washing
       (affinity chromatog. using ionic liqs.)
    Biochemical compounds
    Opioids
    Toxins
    RL: ANT (Analyte); ANST (Analytical study)
       (affinity chromatog, using ionic ligs.)
ΙT
    Addlutinins and Lectins
    Antibodies and Immunoglobulins
    Antigens
    Avidins
    Coenzymes
    DNA
    Enzymes, analysis
    Fatty acids, analysis
    Hormones, animal, analysis
    Nucleic acids
    Oligonucleotides
    Peptides, analysis
    RNA
    Receptors
    RL: ANT (Analyte); CPS (Chemical process); NUU (Other use, unclassified);
    PEP (Physical, engineering or chemical process); ANST (Analytical study);
    PROC (Process); USES (Uses)
        (affinity chromatog. using ionic liqs.)
    Carbohydrates, analysis
```

RL: ANT (Analyte); CPS (Chemical process); PEP (Physical, engineering or

chemical process); ANST (Analytical study); PROC (Process)

```
(affinity chromatog, using ionic ligs.)
     Polymers, analysis
     Proteins
     RL: ANT (Analyte); NUU (Other use, unclassified); ANST (Analytical study);
     USES (Uses)
        (affinity chromatog. using ionic ligs.)
     Hormone receptors
     RL: CPS (Chemical process); PEP (Physical, engineering or chemical
     process); PROC (Process)
        (affinity chromatog. using ionic ligs.)
     Ligands
     RL: CPS (Chemical process); PEP (Physical, engineering or chemical
     process); PROC (Process)
        (affinity chromatog. using ionic liqs.)
тт
    Carbonates, uses
     Fibers
    Fluoropolymers, uses
     Glass, uses
     Nitrates, uses
     Polyamides, uses
     Polycarbonates, uses
     Polvesters, uses
     Polyoxyalkylenes, uses
     Polyphosphates
     Sulfates, uses
     RL: NUU (Other use, unclassified); USES (Uses)
        (affinity chromatog, using ionic ligs.)
     Polymers, uses
     RL: NUU (Other use, unclassified); USES (Uses)
        (co-; affinity chromatog. using ionic liqs.)
     Solvents
       (cosolvents; affinity chromatog. using ionic ligs.)
     Carboxylic acids, uses
     RL: NUU (Other use, unclassified); USES (Uses)
        (esters; affinity chromatog. using ionic ligs.)
     Antibodies and Immunoglobulins
     RL: ANT (Analyte); CPS (Chemical process); NUU (Other use, unclassified);
     PEP (Physical, engineering or chemical process); ANST (Analytical study);
     PROC (Process); USES (Uses)
        (fragments; affinity chromatog, using ionic ligs.)
     Liquids
        (medium; affinity chromatog. using ionic liqs.)
     Halogens
     RL: NUU (Other use, unclassified); USES (Uses)
        (polymer derivs.; affinity chromatog. using ionic ligs.)
     Proteins
     RL: ANT (Analyte); CPS (Chemical process); NUU (Other use, unclassified);
     PEP (Physical, engineering or chemical process); ANST (Analytical study);
     PROC (Process); USES (Uses)
        (recombinant; affinity chromatog. using ionic ligs.)
     Sulfonic acids, uses
     RL: NUU (Other use, unclassified); USES (Uses)
        (salts; affinity chromatog, using ionic ligs.)
     Solids
        (semi-; affinity chromatog, using ionic ligs.)
     Enzymes, biological studies
     RL: BSU (Biological study, unclassified); BIOL (Biological study)
        (substrate; affinity chromatog. using ionic liqs.)
     Proteins
     RL: CPS (Chemical process); PEP (Physical, engineering or chemical
     process); PROC (Process)
        (sugar-binding; affinity chromatog, using ionic ligs.)
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Proteins
     RL: ANT (Analyte); NUU (Other use, unclassified); ANST (Analytical study);
     USES (Uses)
        (surface domains; affinity chromatog, using ionic ligs.)
     Affinity
        (tag; affinity chromatog, using ionic ligs.)
     50-36-2, Cocaine 54-11-5, Nicotine 561-27-3, Heroin
     RL: ANT (Analyte); ANST (Analytical study)
        (affinity chromatog, using ionic ligs.)
     97002-71-6, Morphine dehydrogenase
     RL: CAT (Catalyst use); REM (Removal or disposal); PROC (Process); USES
     (Uses)
        (affinity chromatog, using ionic ligs.)
     58-85-5, Biotin
     RL: CPS (Chemical process); NUU (Other use, unclassified); PEP (Physical,
     engineering or chemical process); PROC (Process); USES (Uses)
        (affinity chromatog, using ionic liqs.)
     288-32-4, Imidazole, uses 7631-86-9, Silica, uses 7732-18-5, Water,
     uses 9002-84-0, Polytetrafluoroethylene 9002-86-2, Polyvinyl chloride
     9002-88-4, Polyethylene 9002-89-5 9003-05-8, Polyacrylamide 9003-05-8D, Polyacrylamide, derivs. 9003-07-0, Polypropylene
     9003-17-2, Polybutadiene 9003-53-6, Polystyrene 9004-34-6, Cellulose, uses 9004-54-0, Dextran, uses 9005-53-2, Lignin, uses 9011-14-7,
     Polymethyl methacrylate 9012-36-6, Agarose 9014-63-5, Xylan
     25322-68-3, Polyethylene glycol 33410-59-2, Polyhema 33410-59-2D,
     Polyhema, derivs.
     RL: NUU (Other use, unclassified); USES (Uses)
        (affinity chromatog, using ionic ligs.)
     76-42-6P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (affinity chromatog. using ionic ligs.)
     12654-97-6, Triazine 14798-03-9, Ammonium, uses 16749-13-6,
     Phosphonium 16969-45-2, Pyridinium
                                             17009-90-4, Imidazolium
     17009-91-5, Pyrazolium 17009-93-7, Pyrazinium 17009-95-9, Pyrimidinium
     17009-97-1, Pyridazinium 37306-44-8, Triazole
     RL: NUU (Other use, unclassified); USES (Uses)
        (cations; affinity chromatog. using ionic ligs.)
RE.CNT 4
              THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD
(1) Crane; US 5092992 A 1992 CAPLUS
(2) Koch, P; WO 2004013612 A 2004 CAPLUS
(3) Merck & Co Inc; EP 0529713 A 1993 CAPLUS
(4) Visser; NATO SCIENCE SERIES, II: MATHEMATICS, PHYSICS AND CHEMISTRY 2003,
    V92, P137 CAPLUS
L13 ANSWER 9 OF 12 CAPLUS COPYRIGHT 2009 ACS on STN
AN
    2005:1090138 CAPLUS
DN
    143:386681
ED
    Entered STN: 12 Oct 2005
     Ionic liquids containing protonated primary, secondary or
     tertiary ammonium ions
IN
    Walker, Adam John
PA
    The University of York, UK
SO
    Brit. UK Pat. Appl., 62 pp.
     CODEN: BAXXDU
DT
    Pat.ent.
LA.
    English
     ICM C07C215-08
TC
     ICS C07C215-12; C07C217-30
     23-4 (Aliphatic Compounds)
     Section cross-reference(s): 45
FAN.CNT 1
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	PATENT			KIN	D	DATE			APPLICATION NO. GB 2005-6984					DATE					
PI	GB 2412912 GB 2412912			В			2005	1012 0711	GB 2005-6984						20050407				
	AU 200 CA 256 WO 200 WO 200	3458 350 9 77	31		A1 A1 A2 A3		2005 2005 2005 2005	1020 1020		AU 2 CA 2 WO 2	005- 005- 005-	2320 2563 GB13	25 458 64		2	0050 0050 0050	407		
	W:	CN, GE, LC, NI, SM,	CO, GH, LK, NO,	CR, GM, LR, NZ,	CU, HR, LS, OM,	CZ, HU, LT, PG,	AU, DE, ID, LU, PH, TR,	DK, IL, LV, PL,	DM, IN, MA, PT,	DZ, IS, MD, RO,	EC, JP, MG, RU,	EE, KE, MK, SC,	EG, KG, MN, SD,	ES, KM, MW, SE,	FI, KP, MX, SG,	GB, KR, MZ, SK,	GD, KZ, NA, SL,		
	RV	AZ, EE, RO,	GH, BY, ES,	KG, FI, SI,	KZ, FR, SK,	MD, GB, TR, TG	RU, GR, BF,	TJ, HU, BJ,	TM, IE, CF,	IS, CG,	BE, IT, CI,	BG, LT, CM,	CH, LU, GA,	CY, MC, GN,	CZ,	DE, PL,	DK, PT,		
	CN 199 EP 180 R:)5131 AT,	BE,			CY,	2007 2007 CZ,	DE,	DK,	EE,	ES,	FI,	FR,	GB,	GR,	0050 0050 HU,	407		
PRAI	JP 200 MX 200 IN 200 KR 200 US 200 GB 200 WO 200						MC, 2007 2007 2007 2007 2007 2004									0050 0061 0061 0061 0070	407 005 103 107 119		
PAT	ENT NO.		CLAS	SS	PATE	NT E	AMIL	Y CL	ASSI	FICA	TION	COD	ES						
	2412912		ICM ICS IPC:	I R	C07C C07C C07C [I,A C07C	215- 215- 0215]; 0	-08 -12; 5-00 007C0 5-00	C07C: [I,C 217-	217-]; (-30 007C0 [I,C]	215- ; C0 215-	08 [7C02	I,A] 17-3 I,A]	; C0 0 [I ; C0	7C02 ,A] 7C02	15-1:			
AU :	AU 2005232025		ECLA IPC: IPCI	A I R	C07C C07C C07C C07C	0217 215/ 0215 0215	217-30 [I,A] 15/40; COT0215/08; COT0215/12; COT0217/30 215-00 [I,C*]; COT00215-40 [I,A] 215-00 [I,C*]; COT00215-40 [I,A]; COT00215-0 ; COT00215-12 [I,A]; COT00215-00 [I,C*];								08				
CA :	2563458	3	IPC:	A. I R	C07C B01J [I,A C07C	215/ 0031]; C	7-30 /40; 1-02 007C0 5-00	C07C: [I,A 215- [I,C	215,]; E 00	301J0 [I,C* :07C0	031-] 215-	04 [40 [I,A]	; C0 ; B0	7C02 1J00	15-4			
WO:	WO 2005097731		ECLA IPC:	A I R	[I,C]; B01J0031-02 [I,A]; B01J0031-04 [I,C]; B01J0031-04 [I,A]; C07C0215-08 [I,A]; C07C0215-1 [I,A]; C07C0215-1 [I,A]; C07C0215-10 [I,C]; C07C0215-20 [I,A] C07C215/40; C07C215/8; C07C215-10 [ICS,7]; C07C0215-10 [ICS,7]; B01J0031-02 [ICS,7];							30 1J00: 215-	31-04						
CN :	1997620)	ECLA IPC:	A I	C07C	215/ 0215	7-30 /40; 5-40 301J0	C07C	215,]; (07C0							0 4		

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TPCR
                        C07C0215-00 [I,C]; C07C0215-40 [I,A]; C07C0215-08
                        [I,A]; C07C0215-12 [I,A]; C07C0217-00 [I,C*];
                        C07C0217-30 [I,A]
                 ECLA
                        C07C215/40; C07C215/08; C07C215/12; C07C217/30
 EP 1805131
                 IPCI
                        C07C0215-40 [I,A]; C07C0215-00 [I,C*]
                 IPCR
                        C07C0215-00 [I,C]; C07C0215-40 [I,A]; C07C0215-08
                        [I,A]; C07C0215-12 [I,A]; C07C0217-00 [I,C*];
                        C07C0217-30 [I,A]
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                        C07C215/40; C07C215/08; C07C215/12; C07C217/30
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                        C07C0215-40 [I.A]; C07C0215-00 [I.C*]; C07C0311-03
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                        C07C0215-00 [I,C]; C07C0215-40 [I,A]; C07C0215-08
                        [I,A]; C07C0215-12 [I,A]; C07C0217-00 [I,C*];
                        C07C0217-30 [I,A]; C07C0311-00 [I,C]; C07C0311-03 [I,A]
                 FTERM
                       4H006/AA01; 4H006/AA03; 4H006/AB80
MX 2006011531
                 IPCI
                        B01J0031-02 [I,C*]; B01J0031-04 [I,C*]; C07C0215-40
                        [I,A]; C07C0215-00 [I,C*]
 IN 2006KN03208 IPCI
                        C07C0215-40 [ICM, 7]; C07C0215-00 [ICS, 7]
 KR 2007031302
                 IPCI
                        C07C0215-40 [I,A]; C07C0215-00 [I,A]
 US 20070185330 IPCI
                        C07C0215-02 [I,A]; C07C0215-00 [I,C*]; C07D0211-02
                        [I,A]; C07D0211-00 [I,C*]
                NCT.
                        546/184.000; 564/281.000
    MARPAT 143:386681
OS.
AB
    The present invention relates to ionic liqs. comprising an anion
     and a cation wherein the cation is a primary, secondary or tertiary
     ammonium ion containing a protonated nitrogen atom. The invention also
     provides processes for the manufacture of ionic liqs. For example,
     N, N-dimethylethanolammonium glycolate (I) was prepared by gradually adding
     glycolic acid to an alc. solution of N,N-dimethylethanolamine; after
     completion and neutralization, the cold alc. solution was filtered, solvent
     removed, then frozen in liquid nitrogen and lyophilized in vacuo. After
     gradually allowing the sample to warm to room temperature, 32.85 g (99% yield)
     of I as a pale vellow liquid was isolated. Preferred ionic liqs.
     contain ethanolammonium, diethanolammonium, N-butyldiethanolammonium,
     N, N-dimethylethanolammonium, N-methylethanolammonium,
    N, N-di(methoxyethyl)ammonium and 1-(3-hydroxypropyl)putrescinium ions as
    amine acid; ammonium ionic liq prepn; primary ammonium ion prepn
    ionic lig; secondary ammonium ion prepn ionic lig;
     tertiary ammonium ion prepn ionic lig
        (enzymic; demonstration of application of ionic ligs, in
        enzymic oxidation of methanol to formaldehyde)
     Green chemistry
       Ionic liquids
        (preparation and methods for manufacture of ionic ligs. containing
        protonated primary, secondary or tertiary ammonium ions)
     Quaternary ammonium compounds, preparation
     RL: IMF (Industrial manufacture); NUU (Other use, unclassified); SPN
     (Synthetic preparation); PREP (Preparation); USES (Uses)
        (preparation and methods for manufacture of ionic ligs. containing
        protonated primary, secondary or tertiary ammonium ions)
     Acids, reactions
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (preparation and methods for manufacture of ionic ligs, containing
        protonated primary, secondary or tertiary ammonium ions)
     Solvents
        (preparation and methods for manufacture of ionic liqs. containing
```

protonated primary, secondary or tertiary ammonium ions for use as

solvent in industrial and com. applications)

RL: RCT (Reactant); RACT (Reactant or reagent)

Amines, reactions

(primary; preparation and methods for manufacture of ionic ligs. containing protonated primary, secondary or tertiary ammonium ions) Carboxvlic acids, uses Sulfonic acids, uses RL: NUU (Other use, unclassified); USES (Uses) (salts, anion component for ionic liquid; preparation and methods for manufacture of ionic ligs. containing protonated primary, secondary or tertiary ammonium ions) Amines, reactions RL: RCT (Reactant); RACT (Reactant or reagent) (secondary; preparation and methods for manufacture of ionic ligs. containing protonated primary, secondary or tertiary ammonium ions) ΙT Amines, reactions RL: RCT (Reactant); RACT (Reactant or reagent) (tertiary; preparation and methods for manufacture of ionic liqs. containing protonated primary, secondary or tertiary ammonium ions) 56-14-4, Succinate, uses 57-60-3, Pyruvate, uses 63-36-5, Salicylate, 71-47-6, Formate, uses 71-50-1, Acetate, uses 71-52-3, Hydrogen carbonate, uses 72-03-7, Propanoate, uses 74-81-7, Octanoate, uses 113-21-3, Lactate, uses 166-44-3, Citrate, uses 149-42-7, Fumarate, uses 149-61-1, Malate 150-43-6, uses 151-33-7, Hexanoate, uses 138-70-5, uses 466-14-8, uses 666-14-8, uses 766-76-7, Benzoate, uses 769-61-9, Mandelate 3342-79-8, Nonanoate 3398-75-2 Decanoate 3715-17-1, Tatrtate, uses 3812-32-6, Carbonate, uses 3398-75-2, 7563-37-3, Heptanoate 7631-42-7, Phenylacetate, uses 10023-74-2, Pentanoate, uses 12627-13-3, Silicate 14066-19-4, Hydrogen phosphate, uses 14066-20-7, Dihydrogen phosphate, uses 14265-44-2, Phosphate, 14477-72-6, Trifluoroacetate ion, uses 14797-55-8, Nitrate, uses 14808-79-8, Sulphate, uses 14874-70-5, Tetrafluoroborate 14996-02-2, Hydrogen sulfate, uses 16053-58-0, Methanesulfonate anion 16887-00-6. Chloride, uses 16919-18-9, Hexafluorophosphate 17121-12-9, Metaphosphate (P40124-) 20461-54-5, Iodide, uses Pantothenate 24959-67-9, Bromide, uses 37181-39-8, Trifluoromethanesulfonate 41824-21-9, Crotonate 44864-55-3 45048-62-2 49681-69-8, Hydrogen tartrate, uses 59561-61-4 86848-98-8 86848-99-9 97901-86-5 98837-98-0 130434-58-1 328238-56-8 866621-22-9 RL: NUU (Other use, unclassified); USES (Uses) (anion component for ionic liquid; preparation and methods for manufacture of ionic ligs. containing protonated primary, secondary or tertiary ammonium ions) 176158-74-0P RL: BSU (Biological study, unclassified); IMF (Industrial manufacture); NUU (Other use, unclassified); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses) (biodegrdn, anal, of ionic liquid; preparation and methods for manufacture of ionic liqs. containing protonated primary, secondary or tertiary ammonium ions) 20740-76-5 22852-66-0, Ethanolamine conjugate acid 26265-71-4 36833-63-3 36833-64-4 65591-62-0 90578-97-5 866567-32-0 866567-33-1 866567-34-2

RL: NUU (Other use, unclassified); USES (Uses) (cation component for ionic liquid; preparation and methods for manufacture of ionic liqs. containing protonated primary, secondary or tertiary ammonium ions) 67-56-1, Methanol, reactions

RL: RCT (Reactant); RACT (Reactant or reagent)

(demonstration of application of ionic liqs. in enzymic

oxidation of methanol to formaldehyde)

50-00-0P, Formaldehyde, preparation

RL: SPN (Synthetic preparation); PREP (Preparation) (demonstration of application of ionic ligs. in enzymic

866568-43-6P

```
oxidation of methanol to formaldehyde)
2471-06-9P 2604-13-9P 2805-17-6P 3178-20-9P 4337-66-0P
                                   16830-40-3P 17618-31-4P
            7487-79-8P
                       16530-72-6P
5988-51-2P
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RL: IMF (Industrial manufacture); NUU (Other use, unclassified); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)

(preparation and methods for manufacture of ionic liqs. containing

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RL: IMF (Industrial manufacture); NUU (Other use, unclassified); SPN
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(Synthetic preparation); PREP (Preparation); USES (Uses)

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RL: IMF (Industrial manufacture); NUU (Other use, unclassified); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)

(preparation and methods for manufacture of ionic ligs. containing protonated primary, secondary or tertiary ammonium ions) 79-14-1, Glycolic acid, reactions 102-79-4, N-Butvldiethanolamine 108-01-0, N.N-Dimethylethanolamine 82113-65-3 RL: RCT (Reactant); RACT (Reactant or reagent) (preparation and methods for manufacture of ionic liqs. containing protonated primary, secondary or tertiary ammonium ions) RE, CNT THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD RE (1) Arizona State Univ: WO 2004114445 A1 CAPLUS (2) Armstrong, D; Anal Chem 2001, V73, P3679 CAPLUS (3) Basf; WO 2004090066 A1 CAPLUS (4) Solvent Innovation; WO 03074494 A1 CAPLUS (5) Staatliches Institut; DD 262042 A1 CAPLUS (6) Studiengesellschaft; WO 03060057 A1 CAPLUS (7) Williams, E; The J of Physical Chem 1977, V81(3) CAPLUS L13 ANSWER 10 OF 12 CAPLUS COPYRIGHT 2009 ACS on STN AN 2004:965647 CAPLUS DN 142:109281 ED Entered STN: 12 Nov 2004 ΤI Cofactor-dependent enzyme catalysis in functionalized ionic AU Walker, Adam J.; Bruce, Neil C. CS CNAP, Department of Biology (Area 8), University of York, York, YO10 5YW, Chemical Communications (Cambridge, United Kingdom) (2004), (22), SO 2570-2571 CODEN: CHCOFS: ISSN: 1359-7345 PB Royal Society of Chemistry DT Journal LA English CC 7-3 (Enzymes) Section cross-reference(s): 16 O.S. CASREACT 142:109281 AR Functionalized, hydrogen-bonding ionic liqs. have been successfully evaluated as media for the performance of cofactor-dependent enzyme catalyzed oxidns.; the effects of incorporating hydroxyl groups into both the cation and anion have been studied and the dependence of activity upon water content has been evaluated. oxidn catalyst enzyme cofactor functionalized ionic solvent; dehydrogenase cofactor functionalized ionic solvent Hydrogen bond Oxidation catalysts (cofactor-dependent enzyme-catalyzed oxidns. in functionalized ionic solvents) Enzymes, biological studies RL: BSU (Biological study, unclassified); CAT (Catalyst use); BIOL (Biological study); USES (Uses) (cofactor-dependent enzyme-catalyzed oxidns. in functionalized ionic solvents) Coenzymes RL: BSU (Biological study, unclassified); NUU (Other use, unclassified); BIOL (Biological study); USES (Uses) (cofactor-dependent enzyme-catalyzed oxidns. in functionalized ionic solvents) Solvents (ionic; cofactor-dependent enzyme-catalyzed oxidns. in functionalized ionic solvents) 467-13-0P, Codeinone RL: BPN (Biosynthetic preparation); BIOL (Biological study); PREP (Preparation)

(NADP-dependent morphine dehydrogenase-catalyzed oxidation in functionalized ionic solvents)

- 97002-71-6, Morphine dehydrogenase
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(NADP-dependent morphine dehydrogenase-catalyzed oxidation in functionalized ionic solvents)

- 24292-60-2
 - RL: BSU (Biological study, unclassified); NUU (Other use, unclassified); BIOL (Biological study); USES (Uses) (NADP-dependent morphine dehydrogenase-catalyzed oxidation in

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9028-53-9, Glucose dehydrogenase 9031-72-5, Alcohol dehydrogenase IT RL: CAT (Catalyst use); USES (Uses) (cofactor-dependent enzyme-catalyzed oxidns. in functionalized

ionic solvents) 7732-18-5, Water, uses

RL: NUU (Other use, unclassified); USES (Uses)

(cofactor-dependent enzyme-catalyzed oxidns. in functionalized ionic solvents)

76-57-3, Codeine 616-47-7 627-30-5 1932-50-9, Potassium glycolate 79917-90-1

RL: RCT (Reactant); RACT (Reactant or reagent) (cofactor-dependent enzyme-catalyzed oxidns, in functionalized

- ionic solvents) 67-64-1, Acetone, reactions 1198-69-2, D-Gluconolactone
- RL: RGT (Reagent); RACT (Reactant or reagent) (cofactor-dependent enzyme-catalyzed oxidns. in functionalized ionic solvents)
- 174501-64-5, 1-Butyl-3-methylimidazolium hexafluorophosphate 227617-70-1, 1-Butyl-2,3-dimethylimidazolium hexafluorophosphate 355011-34-6 444724-05-4 670222-24-9 823179-37-9 RL: NUU (Other use, unclassified); USES (Uses)

(solvent; NADP-dependent morphine dehydrogenase-catalyzed oxidation in functionalized ionic solvents)

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- AN 2004:606558 CAPLUS
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- ED Entered STN: 29 Jul 2004
- ΤТ Ionic liquid solvents for use in enzymic biocatalysis
- IN Bruce, Neil Charles; Walker, Adam John
- PΔ Cambridge University Technical Services Ltd., UK

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SO PCT Int. Appl., 40 pp.
    CODEN: PIXXD2
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    ICS C12P017-18
    16-1 (Fermentation and Bioindustrial Chemistry)
     Section cross-reference(s): 7, 27
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US 20060154328 IPCI C12P0001-00 [I,A]

C12P0007-24 [I,A]; C12P0007-26 [I,A]; C12P0017-18 [I,C*]; C12P0017-18 [I,A] 435/041.000

ECLA C12P001/00; C12P007/04; C12P007/24; C12P007/26; C12P017/18

AB This invention relates to ionic liqs. and their use as solvents in biocatalysis. According to a first aspect of the invention there is provided a method of carrying out an enzyme-catalyzed reaction comprising providing a liquid reaction medium which comprises an ionic liquid including an ion which comprises a functional group selected from the group consisting of alkenyl, hydroxyl, amino, thio, carbonyl and carboxyl groups, providing in the liquid reaction medium an enzyme and a substrate for the enzyme, and allowing reaction of the substrate to occur.

ST ionic liq enzymic biocatalysis

NCL.

IT Oxidation

Reduction

(enzymic; ionic liquid solvents for use in enzymic biocatalysis)

IT Anions

Cations Dissociation constant

Ionic liquids

Zwitterions

(ionic liquid solvents for use in enzymic biocatalysis)

IT 7732-18-5, Water, processes 174501-64-5, BMImPF6 721942-96-7
RL: BCP (Biochemical process); BIOL (Biological study); PROC (Process) (ionic liquid solvents for use in enzymic biocatalysis)

II 53-57-6P, NADPH 53-59-8P, NADP 53-84-9P, NAD 58-68-4P, NAGH
67-63-0P, 2-Propanol, biological studies 67-64-1P, Acetone, biological studies 76-57-3P, Codeine 467-13-0P, Codeinone 2646-71-1P
RL: BCP (Biochemical process); BPN (Biosynthetic preparation); BSU (Biological study, unclassified); RCT (Reactant); BIOL (Biological study);
PREP (Preparation); PROC (Process); RACT (Reactant or reagent)
(ionic liquid solvents for use in enzymic biocatalysis)

IT 9028-12-0, NADP alcohol dehydrogenase 9031-72-5, NAD-dependent alcohol dehydrogenase 97002-71-6, Morphine dehydrogenase RL: BCP (Biochemical process); BSU (Biological study, unclassified); CAT (Catalyst use); BIOL (Biological study); PROC (Process); USES (Uses)

(ionic liquid solvents for use in enzymic biocatalysis) 444724-05-4P

RL: BCP (Biochemical process); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); PROC (Process) (ionic liquid solvents for use in enzymic biocatalysis)

II 67-56-1, Methanol, reactions
RL: BCP (Biochemical process); RCT (Reactant); BIOL (Biological study);
PROC (Process); RACT (Reactant or reagent)

(ionic liquid solvents for use in enzymic biocatalysis)
IT 50-00-0P, Formaldehyde, preparation

RL: BPN (Biosynthetic preparation); BIOL (Biological study); PREP (Preparation)

(ionic liquid solvents for use in enzymic biocatalysis)

IT 355011-34-6P

RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (ionic liquid solvents for use in enzymic biocatalysis)

IT 616-47-7, 1-Methylimidazole 627-30-5, 3-Chloro-1-propanol 16940-81-1,
Hexafluorophosphoric acid 20667-12-3, Silver oxide
RL: RCT (Reactant); RACT (Reactant or reagent)
(ionic liquid solvents for use in enzymic biocatalysis)

IT 721942-97-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(ionic liquid solvents for use in enzymic biocatalysis)

RE.CNT 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD RE

- (1) Anon; WO 0155060 A2 CAPLUS
- (2) Anon: EP 1205555 A1 CAPLUS
- L13 ANSWER 12 OF 12 CAPLUS COPYRIGHT 2009 ACS on STN
- AN 2003:1013019 CAPLUS
- DN 140:253740
- ED Entered STN: 31 Dec 2003
- TI Combined biological and chemical catalysis in the preparation of oxycodone
- AU Walker, Adam J.; Bruce, Neil C.
- CS Institute of Biotechnology, University of Cambridge, Cambridge, CB2 1QT, UK
- SO Tetrahedron (2004), 60(3), 561-568 CODEN: TETRAB; ISSN: 0040-4020
- PB Elsevier Science B.V.
- DT Journal
- LA English
- CC 31-3 (Alkaloids)
- OS CASREACT 140:253740
- AB The opioid oxycodone was produced from codeine, using a combination of chemical and biol. catalysis. The use of novel functionalized ionic ligs. permitted this reaction to be performed in a single solvent.
- ST oxycodone prepn codeine
- IT Ionic liquids
 - (combined biol. and chemical catalysis in preparation of oxycodone)

 T Solvents
 - (ionic liqs.; combined biol. and chemical catalysis in preparation of oxycodone)
- IT 467-13-0P, Codeinone 509-66-0P, Neopinone
 - RL: BPN (Biosynthetic preparation); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant)
 - or reagent)
 - (combined biol. and chemical catalysis in preparation of oxycodone) 76-42-6P, Oxycodone
 - RL: BPN (Biosynthetic preparation); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
 - (combined biol. and chemical catalysis in preparation of oxycodone) 97002-71-6, Morphine dehydrogenase
- RL: CAT (Catalyst use); USES (Uses)
 (combined biol. and chemical catalysis in preparation of oxycodone)
- IT 670222-24-9P
 RL: NUU (Other use, unclassified); SPN (Synthetic preparation); PREP
- (Preparation); USES (Uses)
 (combined biol. and chemical catalysis in preparation of oxycodone)
- T 76-57-3, Codeine 616-47-7, 1-Methyllmidazole 627-30-5, 3-Chloro-1-propanol 1422-07-7, Codeine hydrochloride 1932-50-9,
 - Potassium glycolate RL: RCT (Reactant); RACT (Reactant or reagent)
- (combined biol. and chemical catalysis in preparation of oxycodone)
- RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
- (combined biol. and chemical catalysis in preparation of oxycodone) RE.CNT 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD
- (1) Anon; Ionic liquids in synthesis 2002
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- (3) Bruce, N; Arch Microbiol 1990, V154, P465 CAPLUS
- (4) Bryant, R; Chem Ind 1988, P146 CAPLUS
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(25) Tang, C; PhD Thesis, University of Cambridge 2003
(26) Walker, A; Submitted for publication
(27) Way, W; Basic and clinical pharmacology; 6th ed 1995
(28) Welton, T; Chem Rev 1999, V99, P2071 CAPLUS
=> d his
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              1 S E3
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L2
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L3
              2 S DIMETHYLETHANOLAMMONIUM AND FORMATE
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     FILE 'REGISTRY' ENTERED AT 13:15:11 ON 19 MAR 2009
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L5
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L6
             6 S L5
L7
             56 S (DIMETHYLAMINOETHANOL OR DIMETHYLAMINO ETHANOL) AND (FORMIC O
L8
             0 S IONIC AND L7
L9
             55 S L7 NOT L6
L10
             62 S (DIMETHYLAMINOETHANOL OR DIMETHYLAMINO ETHANOL) AND IONIC
             6 S (DIMETHYLAMINOETHANOL OR DIMETHYLAMINO ETHANOL) AND (IONIC LI
                E WALKER ADAM JOHN/AU
             12 S E2 OR E3
1.13
             12 S L12 AND IONIC
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=> s (dimethylaminoethanol or dimethylamino ethanol) and 113

2798 DIMETHYLAMINOETHANOL

77799 DIMETHYLAMINO

324073 ETHANOL

1061 DIMETHYLAMINO ETHANOL (DIMETHYLAMINO(W)ETHANOL)

L14 0 (DIMETHYLAMINOETHANOL OR DIMETHYLAMINO ETHANOL) AND L13

=> s 59101-30-3 and 113 REG1stRY INITIATED

Substance data SEARCH and crossover from CAS REGISTRY in progress... Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

L16 6 L15

L17 1 L16 AND L13

=> d

L17 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2009 ACS on STN

AN 2005:1090138 CAPLUS

DN 143:386681

TI Ionic liquids containing protonated primary, secondary or tertiary ammonium ions

IN Walker, Adam John

PA The University of York, UK

SO Brit. UK Pat. Appl., 62 pp. CODEN: BAXXDU

DT Patent

LA English

FAN.	PATENT	NO.			KIN	D	DATE			APPL						ATE	
PI	GB 2412 GB 2412				A		2005 2007	1012		GB 2						0050	
	AU 2005						2005			AU 2	005-	2320	25		2	0050	407
	CA 2563						2005			CA 2						0050	
	WO 2005						2005			WO 2						0050	
	WO 2005														_		
		AE,								BB,	BG,	BR,	BW,	BY,	BZ,	CA,	CH,
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		SM,	SY,	ΤJ,	TM,	TN,	TR,	TT,	TZ,	UA,	UG,	US,	UZ,	VC,	VN,	YU,	ZA,
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	EP 1805															0050	
	R:	ΑT,														HU,	IE,
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        JP 2007-506841
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        MX 2006011531
        A 20070326
        MX 2006-11531
        20061005

        IN 2006K03208
        A 20070608
        IN 2006-MX3208
        20061103

        KR 2007031302
        A 20070319
        KR 2006-723342
        20061107

                            A1 20070809
                                                 US 2007-599694
     US 20070185330
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PRAI GB 2004-7908
                             A 20040407
     WO 2005~GB1364
                             W
                                   20050407
OS MARPAT 143:386681
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                ALL CITATIONS AVAILABLE IN THE RE FORMAT
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                  E E2
                1 S E3
     FILE 'CAPLUS' ENTERED AT 13:01:52 ON 19 MAR 2009
                1 S US20070185330/PN
L3
                2 S DIMETHYLETHANOLAMMONIUM AND FORMATE
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      FILE 'REGISTRY' ENTERED AT 13:15:11 ON 19 MAR 2009
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     FILE 'CAPLUS' ENTERED AT 13:16:40 ON 19 MAR 2009
                  S 59101-30-3/REG#
     FILE 'REGISTRY' ENTERED AT 13:18:46 ON 19 MAR 2009
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     FILE 'CAPLUS' ENTERED AT 13:18:47 ON 19 MAR 2009
L6
               6 S L5
L7
               56 S (DIMETHYLAMINOETHANOL OR DIMETHYLAMINO ETHANOL) AND (FORMIC O
L8
                0 S IONIC AND L7
               55 S L7 NOT L6
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               62 S (DIMETHYLAMINOETHANOL OR DIMETHYLAMINO ETHANOL) AND IONIC
L11
                6 S (DIMETHYLAMINOETHANOL OR DIMETHYLAMINO ETHANOL) AND (IONIC LI
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L12
               12 S E2 OR E3
L13
               12 S L12 AND TONIC
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                0 S (DIMETHYLAMINOETHANOL OR DIMETHYLAMINO ETHANOL) AND L13
                  S 59101-30-3/REG# AND L13
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L15
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     FILE 'CAPLUS' ENTERED AT 13:38:11 ON 19 MAR 2009
L16
                6 S L15
L17
                1 S L16 AND L13
=> s 110 and 113
T.18
              0 L10 AND L13
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COST IN U.S. DOLLARS
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FULL ESTIMATED COST 4.49 383.67

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http://www.cas.org/support/stngen/stndoc/properties.html

=> e dimethy	lamino	ethanol/cn
E1	1	DIMETHYLAMINOETHANE HYDROCHLORIDE/CN
E2	1	DIMETHYLAMINOETHANETHIOL S-SULFATE/CN
E3	0>	DIMETHYLAMINOETHANOL/CN
E4	1	DIMETHYLAMINOETHANOL 2-(3-TRIFLUOROMETHYL)PHENOXYNICOTINATE/
		CN
E5	1	DIMETHYLAMINOETHANOL 3-PYRIDINECARBOXYLATE/CN
E6	1	DIMETHYLAMINOETHANOL 4-CHLOROPHENOXYISOBUTYRATE/CN
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E8	1	DIMETHYLAMINOETHANOL ACETATE/CN
E9	1	DIMETHYLAMINOETHANOL ACETYLSALICYLATE/CN
E10	1	DIMETHYLAMINOETHANOL BITARTRATE/CN
E11	1	DIMETHYLAMINOETHANOL CYCLOBUTANECARBOXYLATE/CN
E12	1	DIMETHYLAMINOETHANOL GLUTAMATE/CN
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E3		DIMETHYLAMINO ETHANOL/CN
E4	1	DIMETHYLAMINO ETHOXY DISULFIDE/CN
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E7	1	DIMETHYLAMINO RADICAL/CN
E8	1	DIMETHYLAMINO SALT OF 3', 4'-DICHLOROBENZENESULFONYLISOUREA/C
		N
E9	1	DIMETHYLAMINO SALT OF P-ACETYLAMINOBENZENESULFONYLISOUREA/CN
E10	1	DIMETHYLAMINO (METHYL) SILYLENE/CN
E11	1	DIMETHYLAMINO-1-METHYLETHYL P-CHLOROPHENOXYACETATE/CN
E12	1	DIMETHYLAMINO-2, 4, 5-TRICHLOROBENZOATE/CN

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L20 0 C3H110N/MF

=> s c3h11no/mf

L21 0 C3H11NO/MF

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 TOTAL

 FULL ESTIMATED COST
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 402.12

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FILE COVERS 1907 - 19 Mar 2009 VOL 150 ISS 12 FILE LAST UPDATED: 18 Mar 2009 (20090318/ED)

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http://www.cas.org/legal/infopolicy.html

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s dimethylaminoethanol

L22 2798 DIMETHYLAMINOETHANOL

=> d 1-5

L22 ANSWER 1 OF 2798 CAPLUS COPYRIGHT 2009 ACS on STN

N 2009:236670 CAPLUS

- II Low viscosity liquid curable epoxy resin compositions and their cured products
- IN Kamata, Ami; Sawada, Goro; Maruyama, Isao; Haba, Kazuhiko
- PA Maruzen Oil Co., Ltd., Japan
- SO Jpn. Kokai Tokkyo Koho, 21pp.
- CODEN: JKXXAF

DT Patent

LA Japanese

FAN. CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE		
PI	JP 2009040989	A	20090226	JP 2008-7860	20080117		
PRAI	JP 2007-188569	A	20070719				

- L22 ANSWER 2 OF 2798 CAPLUS COPYRIGHT 2009 ACS on STN
- 2009:236594 CAPLUS AN
- TI Modified polvolefin aqueous dispersions showing good dispersion stability without using emulsifying agents
- TN Kiyosada, Shunji; Oishi, Kei; Nakagiri, Ryuzaburo; Oshita, Shinichi
- PA Seiko PMC Corporation, Japan
- SO Jpn. Kokai Tokkyo Koho, 22pp.
- CODEN: JKXXAF DТ Patent
- LA Japanese
- FAN.CNT 1

1	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE		
	JP 2009040920 JP 2007-208643	A	20090226 20070809	JP 2007-208643	20070809		

- L22 ANSWER 3 OF 2798 CAPLUS COPYRIGHT 2009 ACS on STN
- AN 2009:197674 CAPLUS
- DN 150:228306
- Electric circuit patterns and electrically conducting films, their
- manufacture by printing, and their laminates with cation exchangers Sato, Mutsuko; Sakaguchi, Kaori; Shiraishi, Kinya; Kamoshita, Miyuki
- IN Toyo Ink Mfg. Co., Ltd., Japan PA
- SO Jpn. Kokai Tokkyo Koho, 30pp.
- CODEN: JKXXAF
- Patent
- LA Japanese
- FAN.CNT 1

	PA:	TENT NO.	KIND	DATE	APPLICATION NO.	DATE		
PI PRAI		2009037943 2007-202555	A	20090219 20070803	JP 2007-202555	20070803		

- L22 ANSWER 4 OF 2798 CAPLUS COPYRIGHT 2009 ACS on STN
- AN 2009:173771 CAPLUS
- ΤI Synthesis, characterization and catalytic activity of novel Co(II) and Pd(II)-perfluoroalkylphthalocyanine in fluorous biphasic system; benzyl alcohol oxidation
- AII Ozer, Metin; Yilmaz, Filiz; Erer, Hakan; Kani, Ibrahim; Bekaroglu, Ozer
- CS Department of Chemistry, Marmara University, Istanbul, 34722, Turk.
- so. Applied Organometallic Chemistry (2009), 23(2), 55-61 CODEN: AOCHEX: ISSN: 0268-2605
- PB John Wiley & Sons Ltd.
- DT Journal
- LA English
- RE.CNT 62 THERE ARE 62 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT
- L22 ANSWER 5 OF 2798 CAPLUS COPYRIGHT 2009 ACS on STN
- AN 2009:145165 CAPLUS
- TΤ Synthesis of polyhedral oligosilsesquioxanes containing isocyanate groups in an organic shell of the silsesquioxane core
- Klimenko, N. S.; Gumennaya, M. A.; Shevchuk, A. V.; Dordii, N. K.; AII Shevchenko, V. V.
- Institute of Chemistry of High Molecular Compounds, National Academy of

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Sciences of Ukraine, Kiev, Ukraine
    Dopovidi Natsional noi Akademii Nauk Ukraini (2008), (12), 117-121
SO
    CODEN: DNAUFL; ISSN: 1025-6415
    Vidavnichii Dim "Akademperiodika"
PR
    Journal
DT
LA
    Russian
=> d 1-5 all
L22 ANSWER 1 OF 2798 CAPLUS COPYRIGHT 2009 ACS on STN
    2009:236670 CAPLUS
ED
    Entered STN: 27 Feb 2009
ΤТ
    Low viscosity liquid curable epoxy resin compositions and their cured
    products
TN
    Kamata, Ami; Sawada, Goro; Maruyama, Isao; Haba, Kazuhiko
   Maruzen Oil Co., Ltd., Japan
PA
    Jpn. Kokai Tokkyo Koho, 21pp.
SO
    CODEN: JKXXAF
DT
    Patent
LA
    Japanese
CC
    42-9 (Coatings, Inks, and Related Products)
    Section cross-reference(s): 37
FAN.CNT 1
    PATENT NO.
                       KIND
                              DATE
                                         APPLICATION NO.
    JP 2009040989
                              20090226
                                          JP 2008-7860
                                                                20080117
                        А
PRAT JP 2007-188569
                        Α
                              20070719
CLASS
PATENT NO.
               CLASS PATENT FAMILY CLASSIFICATION CODES
JP 2009040989
                [I,A]; C08G0065-00 [I,C*]; C08L0063-00 [I,A]
                FTERM 4J002/CD021; 4J002/CD051; 4J002/EB118; 4J002/EE059;
                       4J002/EJ019; 4J002/EJ029; 4J002/EL056; 4J002/EN029;
                       4J002/EN109; 4J002/EN138; 4J002/EQ018; 4J002/EU119;
                       4J002/EV298; 4J002/EV319; 4J002/EW178; 4J002/EW179;
                       4J002/EY018; 4J002/FD039; 4J002/FD146; 4J002/FD158;
                       4J002/GH00; 4J002/GH01; 4J002/GJ01; 4J002/GQ01;
                       4J002/GQ05; 4J005/AA09; 4J005/BB02; 4J036/AA01;
                       4J036/AD08; 4J036/AJ09; 4J036/EA01; 4J036/FA10;
                       4J036/FA12; 4J036/GA01; 4J036/GA02; 4J036/GA03;
                      4J036/GA04; 4J036/GA06; 4J036/HA02; 4J036/JA01;
                      4J036/JA06: 4J036/JA07: 4J036/JA15
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        OCH=CH2
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AB The title compns., useful for coatings, inks, adhesives, etc., contain epoxy resins, vinyl ether-containing oxetanes represented by I [Rl = H, Cl-4 alkyl; R2 = (ether-containing) Cl-4 alkylenel, and cationic polymerization initiators. Thus, a composition containing 3,4-epoxycyclohexane-based epoxy resin

Ι

(II; Celloxide 2081) 70, 3-ethyl-3-(vinyloxymethyl)oxetane (III) 30, and

sulfonium salt thermal polymerization initiator (Adeka Opton CP 66) 1 parts showed viscosity 46.6 mPa.s at 23° and cured at 100° for 3 h

and 150° for 4 h to give a test piece showing Tg 87°. A

composition containing II 70, III 30, diaryl iodonium salt photopolymn.

(Irgacure 250) 1, and silicone surface conditioner 1 part was applied on a mild steel plate and irradiated with UV to give a coating showing good adhesion, flat surface with no wrinkle, and pencil hardness (JIS k 5400) H.

ST epoxy resin oxetane liq curable low viscous; epoxycyclohexane sulfonium polymn initiator cured product; ethylvinyloxymethyloxetane liq epoxy resin curable coating

IT Polymerization catalysts

(cationic; low viscosity liquid curable epoxy resin compns. for cured products)

Polyethers

RL: IMF (Industrial manufacture); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses) (epoxy-polyester-; low viscosity liquid curable epoxy resin compns. for

(epoxy-polyester-; low viscosity liquid curable epoxy resin compns. ro cured products)

IT Polyesters

RL: IMF (Industrial manufacture); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)

(epoxy-polyether-; low viscosity liquid curable epoxy resin compns. for cured products)

T Polyethers

RL: IMF (Industrial manufacture); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)

(epoxy; low viscosity liquid curable epoxy resin compns. for cured products)

IT Epoxy resins

RL: POF (Polymer in formulation); USES (Uses)

(low viscosity liquid curable epoxy resin compns. for cured products)
Epoxy resins

RL: IMF (Industrial manufacture); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)

(polyester-polyether-; low viscosity liquid curable epoxy resin compns. for cured products)

IT Epoxy resins

RL: IMF (Industrial manufacture); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)

(polyether-; low viscosity liquid curable epoxy resin compns. for cured products)

IT Onium compounds

Sulfonium compounds

RL: CAT (Catalyst use); USES (Uses)

(polymerization initiators; low viscosity liquid curable epoxy resin compos. for

cured products)

IT Coating materials

(storage-stable; low viscosity liquid curable epoxy resin compns. for cured products)

IT 25068-38-6, Bisphenol A epoxy resin

RL: POF (Polymer in formulation); USES (Uses)

(assumed monomers; low viscosity liquid curable epoxy resin compns. for cured products)

IT 15805-97-7P

RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)

(low viscosity liquid curable epoxy resin compns. for cured products) T 1121544-92-0P 1121544-93-1P 1121544-94-2P

RL: IMF (Industrial manufacture); TEM (Technical or engineered material

```
use); PREP (Preparation); USES (Uses)
        (low viscosity liquid curable epoxy resin compns. for cured products)
     1333-16-0D, Bisphenol F, epoxy resin
     RL: POF (Polymer in formulation); USES (Uses)
        (low viscosity liquid curable epoxy resin compns. for cured products)
     74-86-2, Acetylene 3047-32-3, 3-Ethyl-3-hydroxymethyloxetane
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (low viscosity liquid curable epoxy resin compns. for cured products)
     108-01-0, 2-Dimethylaminoethanol
     RL: TEM (Technical or engineered material use); USES (Uses)
        (low viscosity liquid curable epoxy resin compns. for cured products)
     92-84-2, Phenothiazine 128-37-0, 2,6-Di-tert-butyl-4-methylphenol
     150-76-5, p-Methoxyphenol
     RL: CAT (Catalyst use); USES (Uses)
        (polymerization inhibitor; low viscosity liquid curable epoxy resin compns.
for
       cured products)
     75482-18-7, CPI 100P 87301-62-0, Adeka Opton CP 66 344562-80-7,
     Irgacure 250
     RL: CAT (Catalyst use); USES (Uses)
        (polymerization initiator; low viscosity liquid curable epoxy resin compns.
for
       cured products)
L22 ANSWER 2 OF 2798 CAPLUS COPYRIGHT 2009 ACS on STN
     2009:236594 CAPLUS
AN
ED
     Entered STN: 27 Feb 2009
    Modified polyolefin aqueous dispersions showing good dispersion stability
    without using emulsifying agents
IN
    Kiyosada, Shunji; Oishi, Kei; Nakagiri, Ryuzaburo; Oshita, Shinichi
PA
    Seiko PMC Corporation, Japan
SO
    Jpn. Kokai Tokkyo Koho, 22pp.
    CODEN: JKXXAF
DT
    Patent
LA
    Japanese
CC
    42-10 (Coatings, Inks, and Related Products)
FAN.CNT 1
    PATENT NO.
                       KIND DATE
                                          APPLICATION NO.
                                                                DATE
PI JP 2009040920
                         A
                               20090226
                                          JP 2007-208643
                                                                20070809
                               20070809
PRAI JP 2007-208643
CLASS
PATENT NO.
             CLASS PATENT FAMILY CLASSIFICATION CODES
JP 2009040920 IPCI
                       C08J0003-02 [I,A]; C08L0051-06 [I,A]; C08L0051-00
                       [I,C*]; C08K0005-17 [I,A]; C08K0005-00 [I,C*];
                       C08F0255-04 [I,A]; C08F0255-00 [I,C*]
                 FTERM 4F070/AA13; 4F070/AB08; 4F070/AC12; 4F070/AC36;
                       4F070/AC38; 4F070/AC39; 4F070/AC46; 4F070/AE14;
                       4F070/AE28; 4F070/CA18; 4F070/CB12; 4J002/BN051;
                       4J002/BN061; 4J002/BN091; 4J002/FD206; 4J002/GH01;
                       4J002/GJ01; 4J002/HA06; 4J026/AA11; 4J026/AA12;
                       4J026/AA13; 4J026/BA27; 4J026/CA02; 4J026/FA03;
                       4J026/FA04; 4J026/GA09
    Title compns. comprise (A) modified polyolefins prepared by grafting (a2)
    3-20 parts unsatd. carboxylic acids and (a3) 4.5-40 parts (meth)acrylic
     acid alkyl esters on (a1) 100 parts polyolefins containing ethylene and
     propylene, (B) basic compds., and (C) dispersion media comprising (c1) H2O
     or (c2) mixed solvents containing H2O and ≤50 parts (for 100 parts of
```

A) organic solvents with solubility for H2O ≥2.5% at normal pressure and 20°. Thus, a modified polyolefin prepared from Licocene PP 1602 (ethylene-propylene copolymer), maleic anhydride, and 2-ethylhexyl

acrylate, 2-methyl-2-aminopropanol, and H2O were mixed to give an emulsion showing good storage stability after 1 wk at 40°. Then, the emulsion was applied on a polypropylene sheet to give a coating with

adhesion strength 450 g/cm.

acrylate grafted ethylene propylene copolymer aq dispersion; coating aq ST polyolefin acrylate grafted maleated; amine ag coating acrylate grafted maleated polyolefin; dispersion stability ag coating modified polyolefin

Polyolefins

RL: IMF (Industrial manufacture); POF (Polymer in formulation); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses) (acrylic, graft, maleated; modified polyolefin aqueous dispersions with good dispersion stability and high adhesion strength)

Coating materials IT (emulsions, water-thinned; modified polyolefin aqueous dispersions with good dispersion stability and high adhesion strength)

Amines

Bases

RL: MOA (Modifier or additive use); USES (Uses)

(modified polyolefin aqueous dispersions with good dispersion stability and high adhesion strength)

Alcohols

RL: NUU (Other use, unclassified); USES (Uses)

(solvents; modified polvolefin aqueous dispersions with good dispersion stability and high adhesion strength)

116219-88-6P 556112-73-3P 678991-17-8P 1060720-62-8P, 2-ethylhexyl acrylate-maleic anhydride-Vestoplast 708 graft copolymer 1060720-70-8P 1119199-64-2P 1119199-66-4P 1119199-71-1P

RL: IMF (Industrial manufacture); POF (Polymer in formulation); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)

(modified polyolefin aqueous dispersions with good dispersion stability and high adhesion strength)

108-01-0, Dimethylaminoethanol 124-68-5,

2-Methyl-2-aminopropanol 1310-73-2, Sodium hydroxide 1336-21-6, Ammonium hydroxide

RL: MOA (Modifier or additive use); USES (Uses)

(modified polyolefin aqueous dispersions with good dispersion stability and high adhesion strength)

74-85-1D, Ethylene, graft copolymers with propylene, unsatd. carboxylic acids, and alkyl (meth)acrylates 115-07-1D, Propylene, graft copolymers with ethylene, unsatd. carboxylic acids, and alkyl (meth)acrylates RL: POF (Polymer in formulation); TEM (Technical or engineered material use); USES (Uses)

(modified polyolefin aqueous dispersions with good dispersion stability and high adhesion strength)

67-63-0, Isopropanol 71-36-3, 1-Butanol 71-41-0, 1-Pentanol 78-93-3, Methyl ethyl ketone 111-76-2, Butyl cellosolve 2-Butanol 7732-18-5, Water

RL: NUU (Other use, unclassified); USES (Uses)

(solvents; modified polyolefin aqueous dispersions with good dispersion stability and high adhesion strength)

- L22 ANSWER 3 OF 2798 CAPLUS COPYRIGHT 2009 ACS on STN 2009:197674 CAPLUS
- AN
- DN 150:228306
 - Entered STN: 19 Feb 2009
- Electric circuit patterns and electrically conducting films, their manufacture by printing, and their laminates with cation exchangers
- TN Sato, Mutsuko; Sakaguchi, Kaori; Shiraishi, Kinya; Kamoshita, Miyuki
- PA Toyo Ink Mfg. Co., Ltd., Japan
- SO Jpn. Kokai Tokkyo Koho, 30pp.
 - CODEN: JKXXAF
- DT Patent

LA Japanese

CC 76-14 (Electric Phenomena)

FAN.CNT 1

PATENT NO. KIND DATE APPLICATION NO. DATE PI JP 2009037943 A 20090219 JP 2007-202555 20070803 PRAT JP 2007-202555 20070803 CLASS PATENT NO. CLASS PATENT FAMILY CLASSIFICATION CODES

[I,A]; H01B0001-22 [N,A] FTERM 5G301/DA02; 5G301/DA03; 5G301/DA05; 5G301/DA06; 5G301/DA07; 5G301/DA10; 5G301/DA11; 5G301/DA12;

5G301/DA42; 5G301/DD02; 5G301/DE01; 5G307/FA01; 5G307/FA02; 5G307/FB02; 5G307/FC10; 5G307/GA06; 5G307/GB02; 5G307/GC02

- ΔR Title manufacturing method includes touching elec. conducting materials coated with N and/or S-containing protective layers to cation exchangers. Is also claimed, the manufacturing process by printing with circuit patterns using inks or coatings containing elec. conducting materials on cationic exchange layers. The laminates are useful for an antenna for a noncontact IC medium. The cationic exchange layers expose the elec. conducting materials (e.g., Ag) by releasing the protective layers or exchanging with cations and accelerate film-forming process.
- ST silver circuit pattern printing cation exchanger; surfactant protective layer silver cation exchanger
- Cation exchangers

Laminated materials

Printed circuits

(elec. circuit patterns laminated with cationic exchange layers manufactured by printing)

Films

(elec. conductive; elec. circuit patterns and elec. conducting films, their manufacture by printing, and their laminates with cation exchangers)

Electric conductors

(films; elec. circuit patterns and elec. conducting films, their manufacture by printing, and their laminates with cation exchangers)

copper alloy, nonbase gold alloy, nonbase

iron allov, nonbase

nickel alloy, nonbase palladium alloy, nonbase

platinum alloy, nonbase silver alloy, nonbase

RL: TEM (Technical or engineered material use); USES (Uses) (elec. conductor; elec. circuit patterns laminated with cationic

exchange layers manufactured by printing) 151-21-3, Emal 0, uses 95145-35-0, Gohsenal T 350

RL: TEM (Technical or engineered material use); USES (Uses)

(cationic exchange; elec. circuit patterns laminated with cationic exchange layers manufactured by printing)

7631-86-9, Snowtex 40, uses

RL: TEM (Technical or engineered material use); USES (Uses) (colloidal, cationic exchange; elec. circuit patterns laminated with cationic exchange layers manufactured by printing)

ΤТ 5489-14-5, Silver propionate 7761-88-8, Silver nitrate, reactions RL: RCT (Reactant); RACT (Reactant or reagent)

(elec. circuit patterns laminated with cationic exchange layers manufactured by printing)

7440-22-4P, Silver, uses

RL: IMF (Industrial manufacture); TEM (Technical or engineered material

- use); PREP (Preparation); USES (Uses) (elec. conductor; elec. circuit patterns laminated with cationic
- exchange layers manufactured by printing) 7440-02-0, Nickel, uses 7439-89-6, Iron, uses 7440-05-3, Palladium, 7440-06-4, Platinum, uses 7440-50-8, Copper, uses
- Gold, uses RL: TEM (Technical or engineered material use); USES (Uses) (elec. conductor; elec. circuit patterns laminated with cationic
- exchange layers manufactured by printing) 108-01-0, Dimethylaminoethanol 358377-01-2, Ajisper PB 821
- 375798-26-8, Solsperse 32000
 - - RL: TEM (Technical or engineered material use); USES (Uses) (protective layer; elec. circuit patterns laminated with cationic exchange layers manufactured by printing)
- L22 ANSWER 4 OF 2798 CAPLUS COPYRIGHT 2009 ACS on STN
- ΔN 2009:173771 CAPLUS
- ED Entered STN: 12 Feb 2009
- TΙ Synthesis, characterization and catalytic activity of novel Co(II) and Pd(II)-perfluoroalkylphthalocyanine in fluorous biphasic system; benzyl alcohol oxidation
- ΑU Ozer, Metin; Yilmaz, Filiz; Erer, Hakan; Kani, Ibrahim; Bekaroglu, Ozer
- CS Department of Chemistry, Marmara University, Istanbul, 34722, Turk.
- SO Applied Organometallic Chemistry (2009), 23(2), 55-61 CODEN: AOCHEX; ISSN: 0268-2605
- PB John Wiley & Sons Ltd.
- DT Journal
- LA English

RE.CNT 62

- 25 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
- AB Tetrakis[heptadecafluorononyl] substituted phthalocyanine complexes were prepared by template synthesis from 4-

(heptadecafluorononyloxy)phthalonitrile with Co(CH3COO).24H2O or PdCl2 in 2-N, N-dimethylaminoethanol. The corresponding phthalonitrile

was obtained from heptadecafluorononan-1-ol and 4-nitrophthalonitrile with K2CO3 in DMF at 50 °C. The structures of the compds. were

characterized by elemental anal., FTIR, UV-vis and MALDI-TOF MS

was also tested with different oxidants, such as hydrogen peroxide, m-chloroperoxybenzoic acid, mol. oxygen and oxone in n-hexane-PFMCH.

spectroscopic methods. Metallophthalocyanines are soluble in fluoroalkanes such as perfluoromethylcyclohexane (PFMCH). The complexes were tested as catalysts for benzyl alc. oxidation with tert-butylhydroperoxide (TBHP) in an organic-fluorous biphasic system (n-hexane-PFMCH). The oxidation of benzyl alc.

THERE ARE 62 CITED REFERENCES AVAILABLE FOR THIS RECORD

was found to be the best oxidant for benzyl alc. oxidation since higher conversion and selectivity were observed when this oxidant was used.

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- L22 ANSWER 5 OF 2798 CAPLUS COPYRIGHT 2009 ACS on STN
- AN 2009:145165 CAPLUS
- ED Entered STN: 06 Feb 2009
- Synthesis of polyhedral oligosilsesquioxanes containing isocyanate groups in an organic shell of the silsesquioxane core
- Klimenko, N. S.; Gumennaya, M. A.; Shevchuk, A. V.; Dordii, N. K.; AU Shevchenko, V. V.
- Institute of Chemistry of High Molecular Compounds, National Academy of Sciences of Ukraine, Kiev, Ukraine
- SO Dopovidi Natsional'noi Akademii Nauk Ukraini (2008), (12), 117-121 CODEN: DNAUFL; ISSN: 1025-6415
- PR Vidavnichii Dim "Akademperiodika"

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DT
    Journal
LA
    Russian
CC
    37 (Plastics Manufacture and Processing)
AB
    A mixture of polyhedral oligosilsesquioxanes containing isocyanate groups in
the
     organic shell of a silsesquioxane core (POSS-NCO) is synthesized by the
     reaction of a mixture of polyhedral oligosilsesquioxanes with tertiary
     amine, primary and secondary hydroxylic groups in the organic part of the
     mol. (POSS-M) with excess of tolulene diisocvanate. Its derivative is
     obtained by the reaction of POSS-NCO with N.N-dimethylaminoethanol
     . The structure of the synthesized compds. is characterized by GPC, 1H
     NMR, and IR spectroscopy.
=> d his
     (FILE 'HOME' ENTERED AT 12:57:44 ON 19 MAR 2009)
     FILE 'REGISTRY' ENTERED AT 12:58:22 ON 19 MAR 2009
                E N, N-DIMETHYLETHANOLAMMONIUM FORMATE/CN
                E E2
              1 S E3
     FILE 'CAPLUS' ENTERED AT 13:01:52 ON 19 MAR 2009
              1 S US20070185330/PN
T.3
              2 S DIMETHYLETHANOLAMMONIUM AND FORMATE
     FILE 'CAPLUS' ENTERED AT 13:15:01 ON 19 MAR 2009
     FILE 'REGISTRY' ENTERED AT 13:15:11 ON 19 MAR 2009
T. 4
              2 S 59101-30-3/RN OR 53518-18-6/RN
     FILE 'CAPLUS' ENTERED AT 13:16:40 ON 19 MAR 2009
                S 59101-30-3/REG#
     FILE 'REGISTRY' ENTERED AT 13:18:46 ON 19 MAR 2009
L5
              1 S 59101-30-3/RN
     FILE 'CAPLUS' ENTERED AT 13:18:47 ON 19 MAR 2009
L6
             6 S L5
L7
             56 S (DIMETHYLAMINOETHANOL OR DIMETHYLAMINO ETHANOL) AND (FORMIC O
L8
             0 S IONIC AND L7
L9
             55 S L7 NOT L6
L10
             62 S (DIMETHYLAMINOETHANOL OR DIMETHYLAMINO ETHANOL) AND IONIC
L11
             6 S (DIMETHYLAMINOETHANOL OR DIMETHYLAMINO ETHANOL) AND (IONIC LI
               E WALKER ADAM JOHN/AU
1.12
             12 S E2 OR E3
L13
             12 S L12 AND IONIC
L14
              0 S (DIMETHYLAMINOETHANOL OR DIMETHYLAMINO ETHANOL) AND L13
                S 59101-30-3/REG# AND L13
     FILE 'REGISTRY' ENTERED AT 13:38:11 ON 19 MAR 2009
L15
              1 S 59101-30-3/RN
     FILE 'CAPLUS' ENTERED AT 13:38:11 ON 19 MAR 2009
L16
              6 S L15
              1 S L16 AND L13
T-18
              0 S L10 AND L13
     FILE 'REGISTRY' ENTERED AT 13:39:17 ON 19 MAR 2009
                E DIMETHYLAMINOETHANOL/CN
                E DIMETHYLAMINO ETHANOL/CN
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L19 0 S C3H1101N1/MF
L20 0 S C3H110N/MF
L21 0 S C3H11NO/MF
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FILE 'CAPLUS' ENTERED AT 13:42:24 ON 19 MAR 2009 L22 2798 S DIMETHYLAMINOETHANOL

=> s 113 and 108-01-0

REG1stRY INITIATED

Substance data SEARCH and crossover from CAS REGISTRY in progress... Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

L24 6910 L23

L25 2 L13 AND L24

=> d 1 2 all

L25 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2009 ACS on STN

AN 2007:619447 CAPLUS

DN 147:33228

ED Entered STN: 08 Jun 2007

TI Use of hydroxylammonium salts as ionic liquid solvents for enzyme-catalyzed reactions

IN Walker, Adam John

PA Bionigs Limited, UK

SO PCT Int. Appl., 38pp.

CODEN: PIXXD2 Patent

DT Patent

LA English

CC 45-5 (Industrial Organic Chemicals, Leather, Fats, and Waxes)

Section cross-reference(s): 23

	PAT	ENT :	NO.			KIN	D	DATE		- 1						D	ATE		
I	WO	2007	0633:	063327		A1		20070607		1	WO 2006-GB4503								
		W:	ΑE,	AG,	AL,	AM,	AT,	AU,	AZ,	BA,	BB,	BG,	BR,	BW,	BY,	BZ,	CA,	CH	
			CN,	CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	EG,	ES,	FI,	GB,	GD	
			GE,	GH,	GM,	GT,	HN,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	KE,	KG,	KM,	KN	
			KP,	KR,	KZ,	LA,	LC,	LK,	LR,	LS,	LT,	LU,	LV,	LY,	MA,	MD,	MG,	MK	
			MN,	MW,	MX,	MY,	MZ,	NA,	NG,	NI,	NO,	NZ,	OM,	PG,	PH,	PL,	PT,	RO	
			RS,	RU,	SC,	SD,	SE,	SG,	SK,	SL,	SM,	SV,	SY,	TJ,	TM,	TN,	TR,	TT	
			TZ,	UA,	UG,	US,	UZ,	VC,	VN,	ZA,	ZM,	ZW							
		RW:	AT,	BE,	BG,	CH,	CY,	CZ,	DE,	DK,	EE,	ES,	FΙ,	FR,	GB,	GR,	HU,	ΙE	
			IS,	IT,	LT,	LU,	LV,	MC,	NL,	PL,	PT,	RO,	SE,	SI,	SK,	TR,	BF,	BJ	
			CF,	CG,	CI,	CM,	GA,	GN,	GQ,	GW,	ML,	MR,	NE,	SN,	TD,	TG,	BW,	GH	
			GM,	KE,	LS,	MW,	MZ,	NA,	SD,	SL,	SZ,	TZ,	UG,	ZM,	ZW,	AM,	ΑZ,	BY	
			KG,	KZ,	MD,	RU,	TJ,	TM											
	GB	2437	726			A		2007	1107	(GB 2	006-	2415	7		2	0061	204	
RAI	GB	2005	-247	00		A		2005	1203										
LAS	S																		
PAT	ENT	NO.		CLA	SS	PATE	NT F	AMIL	Y CL	ASSI	FICA	LION	COD	ES					

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[I,C*]; C07C0211-64 [I,A]; C07C0211-00 [I,C*]
                 TPCR
                       C07C0239-00 [I,C]; C07C0239-10 [I,A]; C07C0211-00
                       [I,C]; C07C0211-64 [I,A]; C07C0239-12 [I,A]
                       C07C239/10; C07C239/12
                 ECLA
 GB 2437726
                 IPCI
                       C07C0239-10 [I,A]; C07C0059-06 [I,A]; C07C0059-00
                       [I,C*]; C07C0239-12 [I,A]; C07C0239-00 [I,C*];
                       C07C0311-49 [I,A]; C07C0311-00 [I,C*]; C12P0001-00
                       [I,A]; C12P0007-62 [I,A]
                 IPCR
                       C07C0239-00 [I,C]; C07C0239-10 [I,A]; C07C0059-00
                       [I,C]; C07C0059-06 [I,A]; C07C0239-12 [I,A];
                        C07C0311-00 | I.C1; C07C0311-49 | I.A1; C12P0001-00
                        [I,C]; C12P0001-00 [I,A]; C12P0007-62 [I,C];
                        C12P0007-62 [I,A]
                 ECLA.
                        C07C239/10; C07C239/12
OS
    MARPAT 147:33228
AB
    An ionic liquid comprises cations of the formula R1R2R3N+-OR4,
     where R1, R2, R3 and R4 are each independently selected from hydrogen and
     hydrocarbyl, the ionic liquid containing ≤ 1% of water. The
     ionic ligs. may be used as solvents for chemical or biochem.
     reactions, in particular, for enzyme-catalyzed reactions. Thus,
     N,N-diethylhydroxylammonium acetate (m.p. < -20°, viscosity 12 cP
     at 25°, refractive index 1.414) was prepared by dissolving
     N.N-diethylhydroxylamine (90) and acetic acid (60.06 g) sep. in ethanol
     (250 mL each), and adding the acid solution dropwise to the amine solution over
     1 h, while cooling with ice and stirring.
    hydroxylammonium salt ionic lig solvent enzyme catalyzed
ST
     reaction
     Solvents
        (organic; use of hydroxylammonium salts as ionic liquid solvents
        for enzyme-catalyzed reactions)
     Ionic liquids
        (use of hydroxylammonium salts as ionic liquid solvents for
        enzyme-catalyzed reactions)
     Enzymes, uses
     RL: CAT (Catalyst use); USES (Uses)
        (use of hydroxylammonium salts as ionic liquid solvents for
        enzyme-catalyzed reactions)
     Quaternary ammonium compounds, preparation
     RL: IMF (Industrial manufacture); NUU (Other use, unclassified); PREP
     (Preparation); USES (Uses)
        (use of hydroxylammonium salts as ionic liquid solvents for
        enzyme-catalyzed reactions)
     39004-71-2P, N.N-Diethylhydroxylammonium acetate 939384-89-1P
     939384-90-4P
                  939384-91-5P 939384-93-7P 939384-94-8P 939384-96-0P
     939384-97-1P
     RL: IMF (Industrial manufacture); NUU (Other use, unclassified); PREP
     (Preparation); USES (Uses)
        (use of hydroxylammonium salts as ionic liquid solvents for
        enzyme-catalyzed reactions)
     939384-92-6P
ΙT
     RL: IMF (Industrial manufacture); NUU (Other use, unclassified); RCT
     (Reactant); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
        (use of hydroxylammonium salts as ionic liquid solvents for
        enzyme-catalyzed reactions)
     64-19-7, Acetic acid, reactions
                                     75-75-2, Methanesulfonic acid
     Glycolic acid, reactions 108-01-0, N,N-Dimethylethanolamine
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RL: RCT (Reactant); RACT (Reactant or reagent) (use of hydroxylammonium salts as ionic liquid solvents for

3710-84-7, N,N-Diethylhydroxylamine

121-44-8, Triethylamine, reactions 127-09-3, Sodium acetate

Triflic acid

Hydrochloric acid, reactions

82113-65-3, Bis(trifluoromethylsulfonyl)imide

1493-13-6,

7647-01-0,

7722-84-1, Hydrogen peroxide, reactions

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enzyme-catalyzed reactions)
RE.CNT 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE
(1) Anon
(2) Anon
(3) Anon
(4) Anon
(5) Anon
(6) Anon
(7) Anon
(8) Anon; GAZZ CHIM ITAL 1954, V84, P915
(9) Anon; J AM CHEM SOC 1927, V49, P1539
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L25 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2009 ACS on STN
AN
    2005:1090138 CAPLUS
DN
     143:386681
    Entered STN: 12 Oct 2005
    Ionic liquids containing protonated primary, secondary or
    tertiary ammonium ions
TN
    Walker, Adam John
PA
   The University of York, UK
SO Brit. UK Pat. Appl., 62 pp.
    CODEN: BAXXDU
DT
    Patent
LA
    English
TC
    ICM C07C215-08
     ICS C07C215-12; C07C217-30
     23-4 (Aliphatic Compounds)
     Section cross-reference(s): 45
FAN.CNT 1
                        KIND DATE
    PATENT NO.
                                            APPLICATION NO. DATE
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    GB 2412912
                         A
                               20051012 GB 2005-6984
    GB 2412912
                         В
                               20070711
                     A1 20051020
A1 20051020
A2 20051020
A3 20051124
    AU 2005232025
                                            AU 2005-232025
                                                                     20050407
     CA 2563458
                                            CA 2005-2563458
                                                                    20050407
     WO 2005097731
                                            WO 2005-GB1364
     WO 2005097731
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             GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA,
             NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL,
             SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA,
             ZM. ZW
         RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM,
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             RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML,
             MR, NE, SN, TD, TG
    CN 1997620 A 20070711 CN 2005-80018219
EP 1805131 A2 20070711 EP 2005-735988
                                                                   20050407
                                                                    20050407
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IS, JP 20075325 MX 20060111 IN 2006KN03 KR 20070181 US 20070188 PRAI GB 2004-79 WO 2005-GB	IT, LI 525 531 5208 502 5330	A 20070319 WR 20050407 A 20070407 W 20050407
PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
GB 2412912	ICM ICS IPCI IPCR	C07C215-08 C07C215-12; C07C217-30 C07C0215-00 [I,C]; C07C0215-08 [I,A]; C07C0215-12 [I,A]; C07C0217-00 [I,C]; C07C0217-30 [I,A] C07C0215-00 [I,C]; C07C0215-08 [I,A]; C07C0215-12 [I,A]; C07C0215-40 [I,A]; C07C0215-12
AU 2005232025	ECLA IPCI IPCR	C07C0217-30 [I,A] C07C0215-04; C07C215/08; C07C215/12; C07C217/30 C07C0215-00 [I,C*]; C07C0215-40 [I,A] C07C0215-00 [I,C*]; C07C0215-40 [I,A]; C07C0215-08 [I,A]; C07C0215-12 [I,A]; C07C0217-00 [I,C*]; C07C0217-30 [I,A]
CA 2563458	ECLA IPCI IPCR	C07C215/40; C07C215/08; C07C215/12; C07C217/30 B01J0031-02 [I,A]; B01J0031-04 [I,A]; C07C0215-40 [I,A]; C07C0215-00 [I,C*] C07C0215-00 [I,C]; C07C0215-40 [I,A]; B01J0031-02 [I,C]; B01J0031-02 [I,A]; B01J0031-04 [I,C]; B01J0031-04 [I,A]; C07C0215-08 [I,A]; C07C0215-12 [I,A]; C07C0217-00 [I,C*]; C07C0217-30 [I,A]
WO 2005097731	ECLA IPCI IPCR	COTCC215/40; COTC215/08; COTC215/12; COTC217/30 COTC0215-00 [ICM,7]; COTC0215-40 [ICS,7]; B0IJ0031-04 [ICS,7]; B0IJ0031-02 [ICS,7] COTC0215-00 [I,C*]; COTC0215-08 [I,A]; COTC0215-12 [I,A]; COTC0215-40 [I,A]; COTC0217-00 [I,C*]; COTC0217-30 [I,A]
CN 1997620	ECLA IPCI IPCR	CO7C215/40; CO7C215/08; CO7C215/12; CO7C217/30 CO7C0215-40 [I,A]; CO7C0215-00 [I,C*]; BOIJ0031-04 [I,A]; BOIJ0031-02 [I,A] CO7C0215-00 [I,C]; CO7C0215-40 [I,A]; CO7C0215-08 [I,A]; CO7C0215-12 [I,A]; CO7C0217-00 [I,C*]; CO7C0217-30 [I,A]
EP 1805131	ECLA IPCI IPCR ECLA	COTC215/40; COTC215/08; COTC215/12; COTC217/30 COTC0215-40 [I,A]; COTC0215-00 [I,C*] COTC0215-00 [I,C]; COTC0215-40 [I,A]; COTC0215-08 [I,A]; COTC0215-12 [I,A]; COTC0217-00 [I,C*]; COTC0217-30 [I,A] COTC215/40; COTC215/08; COTC215/12; COTC217/30
JP 2007532525	IPCI IPCR	COTC0215-40 [I,A]; COTC0215-00 [I,C*]; COTC0311-03 [I,A]; COTC0311-00 [I,C*]; COTC0311-00 [I,C*]; COTC0215-00 [I,C]; COTC0215-00 [I,C]; COTC0215-00 [I,A]; COTC0215-00 [I,A]; COTC0217-00 [I,C*]; COTC0217-30 [I,A]; COTC0311-00 [I,C*]; COTC0311-03 [I,A]; COTC0311
MX 2006011531	IPCI	B01J0031-02 [I,C*]; B01J0031-04 [I,C*]; C07C0215-40
IN 2006KN03208 KR 2007031302 US 20070185330	IPCI IPCI IPCI	[I,A]; C07C0215-00 [I,C*] C07C0215-40 [ICM,7]; C07C0215-00 [ICS,7] C07C0215-40 [I,A]; C07C0215-00 [I,A]; C07C0215-02 [I,A]; C07C0215-00 [I,C*]; C07D0211-02 [I,A]; C07D0211-00 [I,C*]
	NCL	546/184.000; 564/281.000

MARPAT 143:386681

OS The present invention relates to ionic liqs. comprising an anion AB and a cation wherein the cation is a primary, secondary or tertiary ammonium ion containing a protonated nitrogen atom. The invention also provides processes for the manufacture of ionic ligs. For example, N, N-dimethylethanolammonium glycolate (I) was prepared by gradually adding glycolic acid to an alc. solution of N,N-dimethylethanolamine; after completion and neutralization, the cold alc. solution was filtered, solvent removed, then frozen in liquid nitrogen and lyophilized in vacuo. After gradually allowing the sample to warm to room temperature, 32.85 g (99% vield) of I as a pale vellow liquid was isolated. Preferred ionic ligs. contain ethanolammonium, diethanolammonium, N-butyldiethanolammonium, N, N-dimethylethanolammonium, N-methylethanolammonium, N, N-di(methoxyethyl)ammonium and 1-(3-hydroxypropyl)putrescinium ions as cations.

amine acid; ammonium ionic liq prepn; primary ammonium ion prepn ST ionic liq; secondary ammonium ion prepn ionic liq; tertiary ammonium ion prepn ionic liq

Oxidation

(enzymic; demonstration of application of ionic ligs. in enzymic oxidation of methanol to formaldehyde)

Green chemistry Ionic liquids

(preparation and methods for manufacture of ionic ligs, containing protonated primary, secondary or tertiary ammonium ions)

Quaternary ammonium compounds, preparation

RL: IMF (Industrial manufacture); NUU (Other use, unclassified); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)

(preparation and methods for manufacture of ionic liqs. containing protonated primary, secondary or tertiary ammonium ions)

Acids, reactions

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation and methods for manufacture of ionic ligs, containing protonated primary, secondary or tertiary ammonium ions)

Solvents

(preparation and methods for manufacture of ionic liqs. containing protonated primary, secondary or tertiary ammonium ions for use as solvent in industrial and com. applications)

Amines, reactions

RL: RCT (Reactant); RACT (Reactant or reagent) (primary; preparation and methods for manufacture of ionic ligs, containing

protonated primary, secondary or tertiary ammonium ions)

Carboxvlic acids, uses

Sulfonic acids, uses

RL: NUU (Other use, unclassified); USES (Uses)

(salts, anion component for ionic liquid; preparation and methods for manufacture of ionic ligs, containing protonated primary, secondary or tertiary ammonium ions)

Amines, reactions

RL: RCT (Reactant); RACT (Reactant or reagent)

(secondary; preparation and methods for manufacture of ionic ligs. containing protonated primary, secondary or tertiary ammonium ions)

Amines, reactions

RL: RCT (Reactant); RACT (Reactant or reagent)

(tertiary; preparation and methods for manufacture of ionic ligs. containing protonated primary, secondary or tertiary ammonium ions)

56-14-4, Succinate, uses 57-60-3, Pyruvate, uses 63-36-5, Salicylate, 71-47-6, Formate, uses 71-50-1, Acetate, uses 71-52-3, Hydrogen uses carbonate, uses 72-03-7, Propanoate, uses 74-81-7, Octanoate, uses 113-21-3, Lactate, uses 126-44-3, Citrate, uses 142-42-7, Fumarate, uses 149-61-1, Malate 150-43-6, uses 151-33-7, Hexanoate, uses 338-70-5, uses 461-55-2, Butanoate, uses 666-14-8, uses 766-76-7,

Benzoate, uses 769-61-9, Mandelate 3342-79-8, Nonanoate 3398-75-2, Decanoate 3715-17-1, Tartrate, uses 3812-32-6, Carbonate, uses 7563-37-3, Heptanoate 7631-42-7, Phenylacetate, uses 10023-74-2, Pentanoate, uses 12627-13-3, Silicate 14066-19-4, Hydrogen phosphate, uses 14066-20-7, Dihydrogen phosphate, uses 14265-44-2, Phosphate, 14477-72-6, Trifluoroacetate ion, uses 14797-55-8, Nitrate, uses 14808-79-8, Sulphate, uses 14874-70-5, Tetrafluoroborate 14996-02-2, Hydrogen sulfate, uses 16053-58-0, Methanesulfonate anion 16887-00-6, Chloride, uses 16919-18-9, Hexafluorophosphate 17121-12-9, Metaphosphate (P40124-) 20461-54-5, Iodide, uses 20938-62-9, Pantothenate 24959-67-9, Bromide, uses 37181-39-8, Trifluoromethanesulfonate 41824-21-9, Crotonate 44864-55-3 45048-62-2 49681-69-8, Hydrogen tartrate, uses 59561-61-4 86848-98-8 86848-99-9 97901-86-5 98837-98-0 130434-58-1 328238-56-8 866621-22-9 RL: NUU (Other use, unclassified); USES (Uses) (anion component for ionic liquid; preparation and methods for manufacture of ionic liqs. containing protonated primary, secondary or tertiary ammonium ions) 176158-74-0P RL: BSU (Biological study, unclassified); IMF (Industrial manufacture); NUU (Other use, unclassified); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses) (biodegrdn, anal, of ionic liquid; preparation and methods for manufacture of ionic liqs. containing protonated primary, secondary or tertiary ammonium ions) 20740-76-5 22852-66-0, Ethanolamine conjugate acid 26265-71-4 36833-64-4 36833-63-3 65591-62-0 90578-97-5 866567-32-0 866567-33-1 866567-34-2 RL: NUU (Other use, unclassified); USES (Uses) (cation component for ionic liquid; preparation and methods for manufacture of ionic ligs. containing protonated primary, secondary or tertiary ammonium ions) 67-56-1, Methanol, reactions RL: RCT (Reactant); RACT (Reactant or reagent) (demonstration of application of ionic liqs. in enzymic oxidation of methanol to formaldehyde) 50-00-0P, Formaldehyde, preparation RL: SPN (Synthetic preparation); PREP (Preparation) (demonstration of application of ionic ligs. in enzymic oxidation of methanol to formaldehyde) 2471-06-9P 2604-13-9P 2805-17-6P 3178-20-9P 4337-66-0P 5988-51-2P 7487-79-8P 16530-72-6P 16830-40-3P 17618-31-4P 17618-32-5P 17863-38-6P 18394-23-5P 20261-59-0P 20475-13-2P 20748-72-5P 21829-52-7P 23251-72-1P, Diethanolamine acetate 23349-61-3P 25859-29-4P 26764-31-8P 28098-03-5P 28129-21-7P, Diethanolamine hydrobromide 29194-47-6P 29867-71-8P 29867-72-9P 29867-75-2P 29868-00-6P 29868-01-7P 29870-14-2P 29870-15-3P 29870-18-6P 29870-19-7P 29870-25-5P 29870-26-6P 29870-27-7P 29870-29-9P 30718-92-4P 30933-06-3P 31086-83-6P 31889-13-1P 35423-90-6P 38491-11-1P 38739-74-1P 49753-18-6P 49753-20-0P 39423-90-6P 38491-11-11-11 38/397-41-F 49/33-18-0F 43/33-20-0F 51264-32-5P 51276-44-9P 53226-33-0P 53562-95-1P 53926-88-7-P 54300-24-2P 55756-39-3P 56409-18-8P 56669-87-5P 57117-29-0P 63517-71-5P 65517-72-6P 64601-03-2P 64601-04-3P 64601-04-3P 67303-52-0P 67384-87-5P 67984-8141-00-4P 68141-46-8P 68391-54-8P,

ΙT

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866568-43-6P
RL: IMF (Industrial manufacture); NUU (Other use, unclassified); SPN
(Synthetic preparation); PREP (Preparation); USES (Uses)
   (preparation and methods for manufacture of ionic liqs. containing
  protonated primary, secondary or tertiary ammonium ions)
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      (Synthetic preparation); PREP (Preparation); USES (Uses)
          (preparation and methods for manufacture of ionic ligs. containing
          protonated primary, secondary or tertiary ammonium ions)
      866570-97-0P 866570-99-2P 866571-01-9P 866571-03-1P
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                        866571-06-4P
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        866571-24-F
        866571-24-F</th
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      RL: IMF (Industrial manufacture); NUU (Other use, unclassified); SPN
      (Synthetic preparation); PREP (Preparation); USES (Uses)
          (preparation and methods for manufacture of ionic ligs, containing
          protonated primary, secondary or tertiary ammonium ions)
      79-14-1, Glycolic acid, reactions 102-79-4, N-Butyldiethanolamine
      108-01-0, N,N-Dimethylethanolamine
                                                     82113-65-3
      RL: RCT (Reactant); RACT (Reactant or reagent)
          (preparation and methods for manufacture of ionic ligs, containing
          protonated primary, secondary or tertiary ammonium ions)
RE.CNT 7
                  THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD
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RE

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               E E2
              1 S E3
    FILE 'CAPLUS' ENTERED AT 13:01:52 ON 19 MAR 2009
             1 S US20070185330/PN
L3
              2 S DIMETHYLETHANOLAMMONIUM AND FORMATE
     FILE 'CAPLUS' ENTERED AT 13:15:01 ON 19 MAR 2009
     FILE 'REGISTRY' ENTERED AT 13:15:11 ON 19 MAR 2009
L4
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L6
             6 S L5
L7
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L8
             0 S IONIC AND L7
             55 S L7 NOT L6
L9
             62 S (DIMETHYLAMINOETHANOL OR DIMETHYLAMINO ETHANOL) AND IONIC
             6 S (DIMETHYLAMINOETHANOL OR DIMETHYLAMINO ETHANOL) AND (IONIC LI
               E WALKER ADAM JOHN/AU
L12
             12 S E2 OR E3
L13
            12 S L12 AND IONIC
L14
             0 S (DIMETHYLAMINOETHANOL OR DIMETHYLAMINO ETHANOL) AND L13
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             1 S L16 AND L13
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L23
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L24
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L25
             2 S L13 AND L24
=> s 108-01-0 and (ionic liquid#)
  REG1stRY INITIATED
Substance data SEARCH and crossover from CAS REGISTRY in progress...
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L27
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       980632 LIQUID#
         13902 IONIC LIQUID#
                 (IONIC(W)LIQUID#)
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L28 ANSWER 1 OF 21 CAPLUS COPYRIGHT 2009 ACS on STN
AN
     2008:1201688 CAPLUS
DN
     149:500958
ED
     Entered STN: 07 Oct 2008
     Density, viscosity and electrical conductivity of
     1-butyl-3-methylimidazolium hexafluorophosphate + monoethanolamine and +
     N, N-dimethylethanolamine
     Geng, Yanfang; Chen, Siliu; Wang, Tengfang; Yu, Dahong; Peng, Changjun;
AU
    Liu, Honglai; Hu, Ying
CS
     Lab for Advanced Material and Department of Chemistry, East China
    University of Science and Technology, Shanghai, 200237, Peop. Rep. China
     Journal of Molecular Liquids (2008), 143(2-3), 100-108
SO
    CODEN: JMLIDT; ISSN: 0167-7322
PB
    Elsevier B.V.
    Journal
DT
LA
    English
CC
    68-6 (Phase Equilibriums, Chemical Equilibriums, and Solutions)
     Section cross-reference(s): 69, 76
AB
     Densities, viscosities and elec. conductivities of ionic liquid
     1-butyl-3-methylimidazolium hexafluorophosphate ([C4mim][PF6]) in
     monoethanolamine (MEA) and N.N-dimethylethanolamine (DMEA) have been determined
     from (288.15 to 323.15) K. The results show that the densities of both
     binary mixts. linearly decrease with increasing temperature  The dependence of
    temperature on the viscosity has been fitted to the Arrhenius equation with
hiah
     precision. A viscosity model based on the equation of state for
     chain-like fluids and a solute aggregation model were used to calculate the
     viscosity of binary mixture The dependence of temperature on the elec.
conductivity has
     also been fitted in the form of Arrhenius equation. The effect of
concentration
     of ionic liquid on the elec. conductivity has been examined using the Walden
     Excess molar volumes and viscosity deviations from a mole fraction average
     have been obtained and fitted to the Redlich-Kister equation.
   butylmethylimidazolium fluorophosphate monoethanolamine
     dimethylethanolamine binary mixt physicochem properties
    Liquid mixtures
        (binary; physicochem. properties of butylmethylimidazolium
        hexafluorophosphate binary mixts. with monoethanolamine and
       dimethylethanolamine)
    Activation energy
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(elec.-conductivity; physicochem. properties of butylmethylimidazolium hexafluorophosphate binary mixts. with monoethanolamine and dimethylethanolamine)

Molar volume

(excess; physicochem. properties of butylmethylimidazolium hexafluorophosphate binary mixts. with monoethanolamine and dimethylethanolamine)

Density

Electric conductivity Ionic liquids Molar conductance

Viscosity

(physicochem, properties of butylmethylimidazolium hexafluorophosphate binary mixts. with monoethanolamine and dimethylethanolamine)

108-01-0, N,N-Dimethylethanolamine 141-43-5, Monoethanolamine, 174501-64-5, 1-Butyl-3-methylimidazolium hexafluorophosphate RL: PEP (Physical, engineering or chemical process); PRP (Properties);

PROC (Process) (physicochem. properties of butylmethylimidazolium hexafluorophosphate binary mixts. with monoethanolamine and dimethylethanolamine)

RE.CNT THERE ARE 48 CITED REFERENCES AVAILABLE FOR THIS RECORD (1) Alan, B; J Electrochem Soc 1997, V144, P84

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- L28 ANSWER 2 OF 21 CAPLUS COPYRIGHT 2009 ACS on STN
- AN 2008:856974 CAPLUS
- DN 149:175904
- ED Entered STN: 17 Jul 2008
- TI Environmentally-friendly quaternary ammonium salts as ionic liquids having low melting point and low viscosity
- IN Ono, Hiroyuki; Fukaya, Yukinobu; Iizuka, Yuki
- PA Tokyo University of Agriculture & Technology, Japan
- SO Jpn. Kokai Tokkyo Koho, 8pp.
- CODEN: JKXXAF
- DT Patent
- LA Japanese
- CC 23-4 (Aliphatic Compounds)

FAN.CNT 1

PATENT N	10.	KIND	DATE	APPLICATION NO.	DATE		
PI JP 20081		A	20080717	JP 2006-350995	20061227		
PRAI JP 2006-	-350995		20061227				
CLASS							
PATENT NO.	CLASS	PATENT	FAMILY CLAS	SIFICATION CODES			

JP 2008162899 IPCI C

- OS CASREACT 149:175904; MARPAT 149:175904
- AB RIRZR3M+CHZCHZOH Y- (R1-R2 = H, C1-3 alkyl; Y = biol.-relevant carboxylate anion) are liquid at ≤90° and are useful as electrolytes, solvents, solubilizers for drugs, etc. Thus, toluene solution of Me2NCHZCH2OH was treated with MeI at 0° for 12 h to give choline iodide, which was dissolved in H2O and passed through a column packed with Amberlite IRA 78 to give choline hydroxide. This was treated with maleic acid at 0° for 12 h to give choline maleate having m.p. 24°.
- ST hydroxyethyl quaternary ammonium biol carboxylate prepn ionic liq; choline maleate prepn low melting point ionic liq
- IT Ionic liquids

(preparation of (hydroxyethyl)quaternary ammonium biol.-relevant carboxylic acid salts as environmentally-friendly quaternary ammonium salts as ionic ligs. having low m.p. and low viscosity)

Quaternary ammonium compounds, preparation

RL: SPN (Synthetic preparation); TEM (Technical or engineered material

use); PREP (Preparation); USES (Uses)

(preparation of (hydroxyethyl)quaternary ammonium biol.-relevant carboxylic acid salts as environmentally-friendly quaternary ammonium salts as ionic ligs. having low m.p. and low viscosity)

IT 64-19-7, Acetic acid, reactions 79-14-1, Glycolic acid, reactions 108-01-0, N,N-Dimethylethanolamine 110-15-6, Succinic acid,

reactions 110-16-7, Maleic acid, reactions

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of (hydroxyethyl)quaternary ammonium biol.-relevant carboxylic acid salts as environmentally-friendly quaternary ammonium salts as

ionic ligs. having low m.p. and low viscosity) 17773-10-3P, Choline iodide RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation of (hydroxyethyl) quaternary ammonium biol.-relevant carboxylic acid salts as environmentally-friendly quaternary ammonium salts as ionic ligs. having low m.p. and low viscosity) 51-84-3P, Choline acetate, preparation 125677-68-1P 143896-90-6P 1039762-54-3P RL: SPN (Synthetic preparation); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses) (preparation of (hydroxyethyl)quaternary ammonium biol.-relevant carboxylic acid salts as environmentally-friendly quaternary ammonium salts as ionic liqs. having low m.p. and low viscosity) 65-85-0D, Benzoic acid, (hydroxyethyl)quaternary ammonium salts 79-09-4D, Propionic acid, (hydroxyethyl)quaternary ammonium salts RL: TEM (Technical or engineered material use); USES (Uses) (preparation of (hydroxyethyl)quaternary ammonium biol.-relevant carboxylic acid salts as environmentally-friendly quaternary ammonium salts as ionic ligs. having low m.p. and low viscosity) L28 ANSWER 3 OF 21 CAPLUS COPYRIGHT 2009 ACS on STN AN 2008:24948 CAPLUS DM 148:247365 Entered STN: 08 Jan 2008 Phase Equilibria and Modeling of Ammonium Ionic Liquid , C2NTf2, Solutions Domanska, Urszula; Marciniak, Andrzej; Krolikowski, Marek AU CS Physical Chemistry Division, Faculty of Chemistry, Warsaw University of Technology, Warsaw, 00-664, Pol. Journal of Physical Chemistry B (2008), 112(4), 1218-1225 SO CODEN: JPCBFK; ISSN: 1520-6106 PB American Chemical Society DT Journal LA English 68-1 (Phase Equilibriums, Chemical Equilibriums, and Solutions) Section cross-reference(s): 23, 65, 69 AB Novel quaternary ammonium ionic liquid, ethyl(2-hydroxyethyl)dimethylammonium bis(trifluoromethylsulfonyl)imide (C2NTf2), has been prepared from N,N-dimethylethanolamine as a substrate. The paper includes a specific basic characterization of the synthesized

water content. The d. of the new compound was measured. The solid-liquid or liquid-liquid phase equilibrium of binary mixts. containing C2NTf2 + water or propan-1-ol, butan-1-ol, hexan-1-ol, octan-1-ol, decan-1-ol, benzene, toluene, hexane, octane, DMSO, and THE were measured by a dynamic method in a wide range of temps. from 230 to 430 K. These data were correlated by means of the nonrandom two-liquid (NRTL) equation utilizing temperature-dependent parameters derived from the solid-liquid or

compound by NMR and the basic thermophys. properties: the m.p., enthalpy of fusion, enthalpy of solid-solid phase transition, glass transition determined by the differential scanning calorimetry (DSC), temperature of decomposition,

liquid-liquid equilibrium

From the solubility results, the neg. value of the partition coefficient of ionic

liquid in binary system octan-1-ol/water (log D) at 298.15 K has been calculated

ST ethylhydroxyethyldimethylammonium salt prepn characterization; org solvent water ethylhydroxyethyldimethylammonium salt binary mixt phase equil

T Quaternary ammonium compounds, properties RI: PEP (Physical, engineering or chemical process); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)

(alkyl; ethyl(hydroxyethyl)dimethylammonium bis(trifluoromethylsulfonyl)imide preparation, characterization and phase equilibrium in its binary mixture with water and organic solvents) Glass transition Ionic liquids Liquid-liquid equilibrium Partition Phase composition Phase transition enthalpy Solid-liquid equilibrium Solubility Thermal decomposition (ethyl(hydroxyethyl)dimethylammonium bis(trifluoromethylsulfonyl)imide preparation, characterization and phase equilibrium in its binary mixture with water and organic solvents) Alkanes, properties Benzenoids RL: PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process) (ethyl(hydroxyethyl)dimethylammonium bis(trifluoromethylsulfonyl)imide preparation, characterization and phase equilibrium in its binary mixture with water and organic solvents) Solvents (organic; ethyl(hydroxyethyl)dimethylammonium bis(trifluoromethylsulfonyl)imide preparation, characterization and phase equilibrium in its binary mixture with water and organic solvents) Alcohols, properties RL: PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process) (primary; ethyl(hydroxyethyl)dimethylammonium bis(trifluoromethylsulfonyl)imide preparation, characterization and phase equilibrium in its binary mixture with water and organic solvents) 71-23-8, 1-Propanol, properties 71-36-3, 67-68-5, DMSO, properties 1-Butanol, properties 71-43-2, Benzene, properties 108-88-3, Toluene, 109-99-9, THF, properties 110-54-3, Hexane, properties 111-27-3, 1-Hexanol, properties 111-65-9, Octane, properties 1-Octanol, properties 112-30-1, 1-Decanol RL: PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process) (ethyl(hydroxyethyl)dimethylammonium bis(trifluoromethylsulfonyl)imide preparation, characterization and phase equilibrium in its binary mixture with. water and organic solvents) 854102-71-9P RL: PEP (Physical, engineering or chemical process); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); PROC (Process) (ethyl(hydroxyethyl)dimethylammonium bis(trifluoromethylsulfonyl)imide preparation, characterization and phase equilibrium in its binary mixture with water and organic solvents)

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bis(trifluoromethylsulfonyl)imide)

RE.CNT 42

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74-96-4, Ethyl bromide 108-01-0, N,N-Dimethylethanolamine 90076-65-6, Lithium bis(trifluoromethanesulfonyl)imide RL: RCT (Reactant); RACT (Reactant or reagent)

(starting material in preparation of ethyl(hydroxyethyl)dimethylammonium

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L28 ANSWER 4 OF 21 CAPLUS COPYRIGHT 2009 ACS on STN
AN 2007:1484110 CAPLUS
DN 148:144204
ED Entered STN: 31 Dec 2007
TΙ
   Process for preparation of ionic liquids with halides
    as anions
    Zhang, Yumei; Wang, Huaping; Zhang, Hongyan; Liu, Weiwei; Wang, Qianghua
TN
PA
   Donghua University, Peop. Rep. China
   Faming Zhuanli Shenqing Gongkai Shuomingshu, 9pp.
SO
    CODEN: CNXXEV
DT
    Patent
LA
    Chinese
     21-2 (General Organic Chemistry)
     Section cross-reference(s): 45
FAN.CNT 1
     PATENT NO.
                        KIND
                              DATE APPLICATION NO. DATE
PI CN 101092399
                        A
                               20071226
                                          CN 2007-10039356
                                                                  20070411
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20070411

PATENT NO. CLASS PATENT FAMILY CLASSIFICATION CODES

PRAI CN 2007-10039356

CLASS

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CN 101092399
               TPCT
                       C07D0233-58 [I,A]; C07D0233-00 [I,C*]; C07D0231-12
                        [I,A]; C07D0231-00 [I,C*]; C07D0213-20 [I,A];
                        C07D0213-00 [I,C*]; C07C0211-63 [I,A]; C07C0211-00
                        [I,C*]; C07C0215-40 [I,A]; C07C0215-00 [I,C*];
                        C07F0009-54 [I,A]; C07F0009-00 [I,C*]
                 IPCR
                       C07D0233-00 [I,C]; C07D0233-58 [I,A]
    CASREACT 148:144204; MARPAT 148:144204
OS
AB
    The method comprises (1) mixing an amine, phosphine, or sulfide compound
     with halogenated hydrocarbon at a molar ratio of 1:1.0-1:1.05; (2)
     allowing to react in reactor at 0.105-0.25 MPa and room temperature-150°C
     for 0.5-20 h under aerating inert gas, decompressing to normal pressure,
     cooling, extracting with 1/5-4/5 volume times Et acetate for 2-3 times,
distilling at
     40-80°C at reduced pressure. The method has advantages of rapid
     reaction, short time, low cost, no pollution to environment, and can be
     used in laboratory synthesis and industrial production With the method, the
prepared
     ionic ligs. can be used as solvent in organic reaction and polymerization
reaction,
     and also used in chemical separation and electrochem. field.
     ionic lig halide anion prepn ammonium phosphonium
     Hydrocarbons, reactions
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (halo; preparation of ionic ligs, with halides as anions)
     Ionic liquids
        (preparation of ionic ligs, with halides as anions)
     Halides
     RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP
     (Preparation)
        (preparation of ionic liqs. with halides as anions)
     4086-73-1P 4317-07-1P 13028-69-8P 65039-08-9P 65039-10-3P
     79917-90-1P
                 85100-77-2P
                               108864-31-9P
                                              1001438-14-7P
                                                               1001438-15-8P
     RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP
     (Preparation)
        (preparation of ionic liqs. with halides as anions)
     74-96-4 96-54-8, N-Methylpyrrole 107-05-1, Allyl chloride
     108-01-0, Dimethylethanolamine 109-65-9, 1-Bromobutane
     109-69-3, 1-Chlorobutane 110-86-1, Pyridine, reactions
     1-Chlorooctane
                     121-44-8, Triethylamine, reactions
                                                         554-70-1,
     Triethylphosphine 616-47-7, N-Methylimidazole
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (preparation of ionic liqs. with halides as anions)
L28 ANSWER 5 OF 21 CAPLUS COPYRIGHT 2009 ACS on STN
AN
    2007:1252115 CAPLUS
DN
    148:223050
ED
    Entered STN: 05 Nov 2007
ΤI
     Solvent extraction of U(VI) by task specific ionic
     liquids bearing phosphoryl groups
ΑU
     Ouadi, Ali; Klimchuk, Olga; Gaillard, Clotilde; Billard, Isabelle
CS
     Institut Pluridisciplinaire Hubert Curien, DRS, ULP, CNRS, IN2P3,
     Strasbourg, 67037, Fr.
     Green Chemistry (2007), 9(11), 1160-1162
SO
     CODEN: GRCHFJ; ISSN: 1463-9262
PB
    Royal Society of Chemistry
DT
    Journal
LA
    English
CC
    68-2 (Phase Equilibriums, Chemical Equilibriums, and Solutions)
    CASREACT 148:223050
```

A novel class of hydrophobic ionic liqs. based on quaternary ammonium cation and bearing phosphoryl groups was synthesized. The preliminary results of U(VI) extraction from aqueous solution into the ionic liquid are

presented.

```
uranyl extn phosphoryl ammonium ionic liq
    Quaternary ammonium compounds, properties
     RL: PEP (Physical, engineering or chemical process); PRP (Properties);
     PROC (Process)
        (alkyl; uranyl solvent extraction of U(VI) by task specific ionic ligs.
        bearing phosphoryl groups)
     Ionic liquids
     Partition
     Solvent extraction
        (uranyl solvent extraction of U(VI) by task specific ionic ligs, bearing
        phosphoryl groups)
     16637-16-4, Uranyl ion(2+)
                                  258273-75-5
     RL: PEP (Physical, engineering or chemical process); PRP (Properties);
     PROC (Process)
        (uranyl solvent extraction of U(VI) by task specific ionic liqs. bearing
        phosphoryl groups)
                   1005000-62-3P
     1005000-61-2P
     RL: PEP (Physical, engineering or chemical process); PRP (Properties); SPN
     (Synthetic preparation); PREP (Preparation); PROC (Process)
        (uranyl solvent extraction of U(VI) by task specific ionic ligs, bearing
        phosphoryl groups)
     108-01-0, 2-(Dimethylamino)ethanol
                                          109-55-7,
     3-(Dimethylamino)-1-propylamine 682-76-8, Dibutyl vinylphosphonate
     819-43-2, Dibutyl chlorophosphate
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (uranyl solvent extraction of U(VI) by task specific ionic ligs. bearing
        phosphoryl groups)
     1013924-26-9P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (uranyl solvent extraction of U(VI) by task specific ionic liqs. bearing
        phosphoryl groups)
RE.CNT
             THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE
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L28 ANSWER 6 OF 21 CAPLUS COPYRIGHT 2009 ACS on STN
AN
     2007:1231612 CAPLUS
DN
     147:553189
ED
    Entered STN: 31 Oct 2007
ΤТ
    Electrochemical-probe type humidity sensor based on room temperature
    ionic liquid
```

TN

Wang, Rong; Zhu, Guoyang

```
PA Shanghai Normal University, Peop. Rep. China
    Faming Zhuanli Shenging Gongkai Shuomingshu, 47pp.
SO
    CODEN: CNXXEV
    Patent
LA Chinese
    79-2 (Inorganic Analytical Chemistry)
CC
FAN.CNT 1
     PATENT NO.
                       KIND DATE APPLICATION NO.
                                                                DATE
                              -----
PI CN 101059476 A
PRAI CN 2007-10041409
                              20071024 CN 2007-10041409
                                                                20070529
                               20070529
CLASS
PATENT NO.
               CLASS PATENT FAMILY CLASSIFICATION CODES
CN 101059476
               IPCI G01N0027-403 [I,A]; G01N0027-26 [I,A]
                IPCR G01N0027-403 [I,C]; G01N0027-403 [I,A]
    The title humidity sensor includes a humidity-sensitive material containing
    room temperature ionic liquid, at least two electrodes (metal electrodes,
carbon
     electrodes or semiconductor electrodes), an electrochem. probe with an
    reversible oxidation-reduction pair as component, a power supply, a
galvanometer,
    a signal circuit, and an ionic liquid carrier; wherein the oxidation-reduction
pair
     is dissolved in ionic liquid and selected from tetracyanoquinodimethane,
     N, N, N', N'-tetramethyl-p-phenylenediamine or benzoquinone, ferrocene,
     potassium ferricyanide, etc., and derivs. thereof; and the room temperature
     ionic liquid is selected from alkylimidazole, alkylpyridine, quaternary
     ammonium salt, quaternary phosphonium salt, or benzimidazole ionic liqs.
     The inventive humidity sensor has the advantages of stable performance,
    high sensitivity, simple structure, and low cost.
    humidity sensor electrochem probe ionic liq
ST
ΙT
    Electric current
     Electrochemistry
     Gas analysis
     Humidity
     Hygrometers
       Ionic liquids
        (electrochem.-probe type humidity sensor based on room temperature ionic
        liquid)
    Phosphonium compounds
     Pyridinium compounds
     Quaternary ammonium compounds, uses
     RL: IMF (Industrial manufacture); TEM (Technical or engineered material
     use); PREP (Preparation); USES (Uses)
        (electrochem.-probe type humidity sensor based on room temperature ionic
        liquid)
    Metalloporphyrins
     RL: TEM (Technical or engineered material use): USES (Uses)
        (electrochem.-probe type humidity sensor based on room temperature ionic
        liquid)
    Onium compounds
     RL: IMF (Industrial manufacture); TEM (Technical or engineered material
     use); PREP (Preparation); USES (Uses)
        (imidazolium compds.; electrochem.-probe type humidity sensor based on
```

room temperature ionic liquid)

143314-16-3P, 1-Ethyl-3-methylimidazolium tetrafluoroborate
174501-64-5P, 1-Butyl-3-methyl imidazolium hexafluorophosphate
186088-50-6P, N-Butylpyridinium hexafluorophosphate
203389-28-0P,
N-Butylpyridinium tetrafluoroborate
244193-56-4P,
1-Decyl-3-methylimidazolium tetrafluoroborate
324575-10-2P
384347-07-3P 547718-93-4P 849223-61-6P 849223-64-9P 855788-71-5P

```
RL: IMF (Industrial manufacture); TEM (Technical or engineered material
     use); PREP (Preparation); USES (Uses)
       (electrochem.-probe type humidity sensor based on room temperature ionic
        liquid)
    74-88-4, Iodo methane, reactions 74-96-4, Bromoethane 75-75-2,
    Methanesulfonic acid 102-71-6, Triethanolamine, reactions 104-15-4,
     p-Methyl benzene sulfonic acid, reactions 108-01-0, N,
    N-Dimethyl ethanolamine 109-65-9, 1-Bromobutane 110-86-1, Pyridine,
     reactions 111-42-2, Diethanolamine, reactions 111-83-1, 1-Bromooctane
     112-29-8, 1-Bromodecane 112-71-0, 1-Bromotetradecane 616-47-7,
     N-Methyl imidazole 998-40-3 1120-71-4, 1, 3-Propane sultone
     1493-13-6, Trifluoromethanesulfonic acid 1633-83-6, 1,4-Butane sultone
     7035-68-9, 1-Ethyl benzimidazole 7664-93-9, Sulfuric acid, reactions 16872-11-0, Tetrafluoroboric acid 17084-13-8, Potassium
     hexafluorophosphate 90076-65-6, Lithium bis(trifluoromethane
     sulfonimide)
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (electrochem.-probe type humidity sensor based on room temperature ionic
       liquid)
     874-80-6P, N-Butvl pyridinium bromide 1702-42-7P,
     Tributylmethylphosphonium iodide 2534-66-9P, N-Octyl pyridinium bromide
     3115-68-2P, Tetrabutylphosphonium bromide 15193-40-5P,
     Tributyltetradecylphosphonium bromide 38880-58-9P 65039-08-9P,
     1-Ethyl-3-methyl imidazolium bromide 80297-71-8P
                                                       85100-77-2P.
     1-Butyl-3-methyl imidazolium bromide 188589-32-4P,
1-Decyl-3-methylimidazolium bromide 288322-16-7P 849223-59-2P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
       (electrochem.-probe type humidity sensor based on room temperature ionic
       liquid)
     100-22-1, N,N,N'N'-Tetramethyl p-phenylene diamine 102-54-5, Ferrocene
     106-51-4, 1,4-Benzoquinone, uses 574-93-6, Phthalocyanine 1518-16-7
     7440-44-0, Carbon, uses 13746-66-2, Potassium ferricyanide 956699-78-8
     RL: TEM (Technical or engineered material use); USES (Uses)
       (electrochem.-probe type humidity sensor based on room temperature ionic
       liquid)
L28 ANSWER 7 OF 21 CAPLUS COPYRIGHT 2009 ACS on STN
AN 2007:1218237 CAPLUS
DN 147:541494
ED Entered STN: 29 Oct 2007
TI Process for preparation of ionic liquids having two
    functional groups
IN Wang, Rong; Zhu, Guoyang; Liu, Guohua; Wu, Xiagin; Dai, Livi
   Shanghai Normal University, Peop. Rep. China
SO Faming Zhuanli Shenging Gongkai Shuomingshu, 14pp.
    CODEN: CNXXEV
   Patent
    Chinese
     23-4 (Aliphatic Compounds)
     Section cross-reference(s): 45
FAN.CNT 1
                              DATE APPLICATION NO. DATE
     PATENT NO.
                       KIND
PI CN 101058552 A
PRAI CN 2006-10025808
                              20071024 CN 2006-10025808 20060418
                              20060418
CLASS
PATENT NO. CLASS PATENT FAMILY CLASSIFICATION CODES
```

TT

PA

DT

LA

[I,A]; C07C0303-00 [I,C*]

C07C0309-00 [I,C]; C07C0309-02 [I,A] TPCR

- OS CASREACT 147:541494; MARPAT 147:541494
- AB This invention pertains to a method for producing ionic ligs, having two functional groups with general formula of

R1R2(R3OCH2CH2)N+(CH2)3SO3H•R4SO3- [wherein R1 and R2 = independently H, alkyl, aryl, etc.; R3 = H, (un)substituted alkyl, or aryl; R4 = alkyl, alkenyl, aryl, heteroaryl, or OH|. The preparation of title ionic liquid comprises reacting hydroxvalkylamine or its derivs, with sultone to obtain corresponding inner salt compds., then mixing with organic acid or inorg. acid at molar ratio of 1: 1 at 50-85 °C, and vacuum drying to

obtain the product. The title ionic liquid has stability in water and atmospheric,

moderate viscosity, low cost, and can be used widely in catalysis and extraction, and can be modified or solidified further by inducing hydroxy and sulfonic groups.

- ammonium sulfonic acid prepn ionic liq
- ΙT Ionic liquids
- (preparation of ionic ligs. having two functional groups)
- IT 38880-58-9P 43192-68-3P 80297-71-8P 88992-91-0P 956719-65-6P 956719-75-8P 956719-80-5P

RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation of ionic ligs. having two functional groups)

- 956699-81-3P 956699-82-4P 956699-83-5P 956699-85-7P 956699-86-8P 956699-87-9P 956719-62-3P 956719-69-0P 956719-73-6P 956719-78-1P 956719-83-8P
 - RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
- (preparation of ionic ligs. having two functional groups)
- 68-11-1, reactions 75-75-2, Methanesulfonic acid 79-10-7, 2-Propenoic acid, reactions 102-71-6, reactions 104-15-4, Tosic acid, reactions 107-99-3 108-01-0 108-95-2, Phenol, reactions 111-42-2, reactions 1120-71-4 1493-13-6, Trifluoromethanesulfonic acid 1633-83-6

RL: RCT (Reactant); RACT (Reactant or reagent)

- (preparation of ionic ligs. having two functional groups)
- 7664-93-9, Sulfuric acid, reactions RL: RGT (Reagent); RACT (Reactant or reagent)

(preparation of ionic ligs, having two functional groups)

- L28 ANSWER 8 OF 21 CAPLUS COPYRIGHT 2009 ACS on STN
- AN 2007:1217631 CAPLUS
- DN 147:553183
- ED Entered STN: 29 Oct 2007
- ΤТ Amperometric humidity sensing device based on room-temperature ionic liquid
- IN Wang, Rong; Zhu, Guoyang
- PA Shanghai Normal University, Peop. Rep. China
- Faming Zhuanli Shenging Gongkai Shuomingshu, 48pp. SO CODEN: CNXXEV
 - Patent
- DT
- LA Chinese
- 79-2 (Inorganic Analytical Chemistry) Section cross-reference(s): 59

FAN CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI CN 101059475	A	20071024	CN 2007-10041408	20070529
PRAI CN 2007-10041408		20070529		
CLASS				

PATENT NO. CLASS PATENT FAMILY CLASSIFICATION CODES

```
IPCI G01N0027-403 [I,A]; G01N0027-26 [I,A]
CN 101059475
                IPCR G01N0027-403 [I,C]; G01N0027-403 [I,A]
    The title amperometric humidity sensing device comprises a
    humidity-sensing element having a room-temperature ionic liquid and an
    electrochem. probe, a signal amplification circuit, a detection loop, a
    reference loop, a gas system, and display controlling system, wherein humidity
    is detected by charge current of the humidity-sensing element and reaction
    current of the electrochem, probe. The room-temperature ionic liquid can be
one
    or more selected from alkylimidazole, alkylpyridine, quaternary ammonium
    salt, quaternary phosphonium salt, and benzimidazole ionic ligs. The
    electrochem. probe can be redox pair, such as
    tetramethyl-p-phenylenediamine, benzoquinone, ferrocene, etc., and derivative
    thereof, dissolved in the room-temperature ionic liquid. The inventive
    amperometric humidity sensing device has simple structure, good
    interference resistance, large responding signal linear range, good
    interchangeability, low cost, stable performance, and high sensitivity.
    amperometric humidity sensing device ionic liq
IΤ
    Sulfonic acids, uses
    RL: IMF (Industrial manufacture); TEM (Technical or engineered material
    use); PREP (Preparation); USES (Uses)
       (alkanesulfonic, salts; amperometric humidity sensor based on
       room-temperature ionic liquid)
    Electric current
    Electrochemistry
    Gas analysis
    Humidity
    Hvarometers
      Ionic liquids
        (amperometric humidity sensor based on room-temperature ionic liquid)
    Phosphonium compounds
    Pyridinium compounds
    Quaternary ammonium compounds, uses
    RL: IMF (Industrial manufacture); TEM (Technical or engineered material
    use); PREP (Preparation); USES (Uses)
        (amperometric humidity sensor based on room-temperature ionic liquid)
    Metallophthalocyanines
    Metalloporphyrins
    RL: TEM (Technical or engineered material use); USES (Uses)
        (amperometric humidity sensor based on room-temperature ionic liquid)
    Onium compounds
    RL: IMF (Industrial manufacture); TEM (Technical or engineered material
    use); PREP (Preparation); USES (Uses)
        (imidazolium compds.; amperometric humidity sensor based on room-temperature
        ionic liquid)
    100-22-1, N.N.N'N'-Tetramethyl p-phenylene diamine
                                                       102-54-5, Ferrocene
    106-51-4, 1,4-Benzoquinone, analysis 1518-16-7 13746-66-2, Potassium
    ferricyanide 13943-58-3, Potassium ferrocyanide
                                                      956699-78-8
    RL: ARU (Analytical role, unclassified); PRP (Properties); ANST
    (Analytical study)
        (amperometric humidity sensor based on room-temperature ionic liquid)
    143314-16-3P, 1-Ethyl-3-methylimidazolium tetrafluoroborate
    174501-64-5P, 1-Butyl-3-methyl imidazolium hexafluorophosphate
    186088-50-6P, N-Butylpyridinium hexafluorophosphate
    N-Butylpyridinium tetrafluoroborate 244193-56-4P,
    1-Decyl-3-methylimidazolium tetrafluoroborate 324575-10-2P
    855788-71-5P
                                               956699-83-5P 956699-85-7P
    956699-86-8P 956699-87-9P 956699-88-0P
    RL: IMF (Industrial manufacture); TEM (Technical or engineered material
    use); PREP (Preparation); USES (Uses)
```

```
(amperometric humidity sensor based on room-temperature ionic liquid)
    74-88-4, Iodo methane, reactions 74-96-4, Bromoethane 75-75-2,
    Methanesulfonic acid 102-71-6, Triethanolamine, reactions 104-15-4,
    p-Methyl benzene sulfonic acid, reactions 108-01-0, N,
    N-Dimethyl ethanolamine 109-65-9, 1-Bromo-butane 110-86-1, Pyridine,
    reactions 111-42-2, Diethanolamine, reactions 111-83-1, 1-Bromo-octane
    112-29-8, 1-Bromo-decane 112-71-0, 1-Bromo-tetradecane 616-47-7,
    N-Methyl imidazole 998-40-3 1120-71-4, 1, 3-Propane sultone
    1493-13-6, Trifluoromethanesulfonic acid 1633-83-6, 1, 4-Butane sultone
    7035-68-9, 1-Ethyl benzimidazole 7664-93-9, Sulfuric acid, reactions
    16872-11-0, Tetrafluoroboric acid 17084-13-8, Potassium
    hexafluorophosphate 90076-65-6, Lithium bis(trifluoromethane
    sulfonimide)
    RL: RCT (Reactant); RACT (Reactant or reagent)
       (amperometric humidity sensor based on room-temperature ionic liquid)
    874-80-6P, N-Butyl pyridinium bromide 1702-42-7P,
    Tributylmethylphosphonium iodide 2534-66-9P, N-Octyl pyridinium bromide
    3115-68-2P, Tetrabutylphosphonium bromide 15193-40-5P,
    Tributyltetradecylphosphonium bromide 38880-58-9P 58431-91-7P
    65039-08-9P, 1-Ethyl-3-methyl imidazolium bromide 80297-71-8P
    85100-77-2P, 1-Butyl-3-methyl imidazolium bromide
                                                      188589-32-4P,
    1-Decv1-3-methylimidazolium bromide 849223-59-2P
    RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
    (Reactant or reagent)
       (amperometric humidity sensor based on room-temperature ionic liquid)
L28 ANSWER 9 OF 21 CAPLUS COPYRIGHT 2009 ACS on STN
    2007:1150094 CAPLUS
AN
DN
    147:502043
    Entered STN: 12 Oct 2007
ED
TI Preparation of ionic liqs. from cycloalkane/benzene carboxylic acids and
    tertiary amines or quaternary ammonium hydroxides
IN
    Zhang, Suojiang; Yu, Yinghao; Yao, Hongwei
    Institute of Process Engineering, Chinese Academy of Sciences, Peop. Rep.
PA
    China
SO
    Faming Zhuanli Shenqing Gongkai Shuomingshu, 6pp.
    CODEN: CNXXEV
DT
    Patent
LA
   Chinese
CC
    24-5 (Alicyclic Compounds)
    Section cross-reference(s): 25
FAN.CNT 1
    PATENT NO.
                       KIND
                             DATE
                                         APPLICATION NO.
PI CN 101050185
                       A
                              20071010 CN 2007-10099180
                                                              20070516
PRAI CN 2007-10099180
                              20070516
CLASS
PATENT NO. CLASS PATENT FAMILY CLASSIFICATION CODES
CN 101050185
                IPCI
                      C07C0211-62 [I,A]; C07C0211-00 [I,C*]; C07F0009-44
                       [I,A]; C07F0009-00 [I,C*]
                IPCR C07C0211-00 [I,C]; C07C0211-62 [I,A]
os
    CASREACT 147:502043; MARPAT 147:502043
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GI

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Ionic ligs. I [wherein A = 5/6-membered ring skeleton; n = 1-5; R = alkyl;
AB
    when R1 = H, R2 - R4 = alkyl or substituted OH, otherwise R1 - R4 = alkyl,
    (un) substituted OH or aryl] were prepared in one step from the corresponding
    carboxylic acids and tertiary amines or quaternary ammonium hydroxides.
    For instance, neutralization of cyclohexanecarboxylic acid with
    benzyltrimethylammonium hydroxide in methanol at 20°C for 22 h gave
    benzyltrimethylammonium cyclohexanecarboxylate. The obtained ionic liquid
    has high electrocond., high heat stability, and high electrochem.
    stability (no data).
    ionic liq prepn carboxylic acid quaternary ammonium hydroxide
    neutralization; cycloalkanecarboxylic benzoic acid tertiary amine ionic
    liq prepn
тт
    Quaternary ammonium compounds, reactions
    RL: RCT (Reactant); RACT (Reactant or reagent)
        (hydroxides; preparation of ionic liqs. from cycloalkane/benzene carboxylic
       acids and tertiary amines or quaternary ammonium hydroxides)
    Ionic liquids
    Neutralization
        (preparation of ionic ligs. from cycloalkane/benzene carboxylic acids and
       tertiary amines or quaternary ammonium hydroxides)
    Carboxvlic acids, reactions
    RL: RCT (Reactant); RACT (Reactant or reagent)
        (preparation of ionic ligs. from cycloalkane/benzene carboxylic acids and
       tertiary amines or quaternary ammonium hydroxides)
    Amines, reactions
    RL: RCT (Reactant); RACT (Reactant or reagent)
        (tertiary; preparation of ionic liqs. from cycloalkane/benzene carboxylic
       acids and tertiary amines or quaternary ammonium hydroxides)
    Quaternary ammonium compounds, preparation
    RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (tetraalkyl; preparation of ionic ligs. from cycloalkane/benzene carboxylic
       acids and tertiary amines or quaternary ammonium hydroxides)
    50-78-2, 2-Acetoxybenzoic acid 56-13-3 65-85-0, Benzoic acid,
    reactions
               69-72-7, Salicylic acid, reactions
                                                    75-59-2.
    Tetramethylammonium hydroxide 77-98-5, Tetraethylammonium hydroxide
    83-44-3, Deoxycholic acid 91-66-7, N,N-Diethylaniline
    Cyclohexanecarboxylic acid 98-94-2 99-97-8,
    N,N-Dimethyl-4-methylaniline 100-37-8, N,N-Diethylethanolamine
    100-85-6, Benzyltrimethylammonium hydroxide 102-69-2, Tripropylamine
    102-82-9, Tributylamine 108-01-0, N,N-Dimethylethanolamine
    108-16-7, N,N-Dimethylisopropanolamine 121-69-7, N,N-Dimethylaniline,
    reactions
               123-41-1, Choline hydroxide
                                             127-19-5, Dimethylacetamide
    471-53-4, 18-β-Glycyrrhetinic acid 514-10-3, Abietic acid
    546-18-9, 5B-Cholanic acid
                                590-78-3 1123-25-7,
    1-Methyl-1-cyclohexanecarboxylic acid 1836-42-6, Benzyltriethylammonium
    hydroxide 1987-53-7 2052-49-5, Tetrabutylammonium hydroxide
    3179-63-3, N,N-Dimethylpropanolamine
                                          3400-45-1, Cyclopentanecarboxylic
           4499-86-9, Tetrapropylammonium hydroxide 4656-13-7 7087-68-5,
    Diisopropylethylamine
                           14898-63-6, Dodecyltrimethylammonium hydroxide
    29960-45-0, Cyclopentenecarboxylic acid
                                             35675-84-4,
    Methyltrioctylammonium hydroxide 38792-89-1
    Dicyclohexylacetic acid
    RL: RCT (Reactant); RACT (Reactant or reagent)
        (preparation of ionic liqs. from cycloalkane/benzene carboxylic acids and
       tertiary amines or quaternary ammonium hydroxides)
    2016-36-6P
                 15032-34-5P
                               955108-09-5P
                                             955108-12-0P
```

RL: SPN (Synthetic preparation); PREP (Preparation)

tertiary amines or quaternary ammonium hydroxides)

(preparation of ionic liqs. from cycloalkane/benzene carboxylic acids and

- IT 64-17-5, Ethanol, uses 67-56-1, Methanol, uses 67-63-0, Isopropanol, uses 67-64-1, Acetone, uses 110-82-7, Cyclohexane, uses 7732-18-5, Water, uses
- RL: NUU (Other use, unclassified); USES (Uses)

(solvent; preparation of ionic liqs. from cycloalkane/benzene carboxylic acids and tertiary amines or quaternary ammonium hydroxides)

- L28 ANSWER 10 OF 21 CAPLUS COPYRIGHT 2009 ACS on STN
- AN 2007:1016184 CAPLUS
- DN 147:486138
- ED Entered STN: 11 Sep 2007
- TI Choline derivative-based ionic liquids
- AU Pernak, Juliusz; Syguda, Anna; Mirska, Ilona; Pernak, Anna; Nawrot, Jan; Pradzynska, Aleksandra; Griffin, Scott T.; Rogers, Robin D.
- CS Poznan University of Technology, Poznan, Pol.
- SO Chemistry--A European Journal (2007), 13(24), 6817-6827, S6817/1-S6817/9 CODEN: CEUJED; ISSN: 0947-6539
- PB Wiley-VCH Verlag GmbH & Co. KGaA
- DT Journal
- LA English
- CC 23-4 (Aliphatic Compounds)
 - Section cross-reference(s): 1, 5, 10, 63, 75, 76
- OS CASREACT 147:486138
- AB A total of sixty-three choline derivative-based ionic liqs.

 RIOCH2CH2N+Me2CH2OR2 X- (R1 = H, MeCO, n-C9H19CO; R2 = Et, n-Pr, n-hexyl, n-decyl, cyclododecyl, etc.) (I) in the forms of chlorides, acesulfamates,
 - and bis(trifluoromethylsulfonyl)imides have been prepared and their phys. properties (d., viscosity, solubility, and thermal stability) have been

determined

Thirteen of these salts are known chlorides: precursors to the 26 water-soluble acesulfanates, 12 acesulfanates only partially miscible with water, and 12 water-insol. imides. The crystal structures for I (Rl = H; R2 = n-undecyl, cyclododecyl; X = Cl) were determined by X-ray anal. The antimicrobial (cocci, rods, and fungi) activities of the new hydrophilic acesulfanate-based ILs were measured and 12 of the compds. were found to be active. The alkowymethyl-2-hydroxyethyl)dimethylammonium acesulfanates have been shown to be insect feeding deterrents and thus open up a new generation of synthetic deterrents based on ionic liqs. The alkowymethyl(2-decanoyloxyethyl)dimethylammonium

bis(trifluoromethylsulfonyl)imides have also been shown to act as

fixatives for soft tissues and can furthermore be used as substitutes for formalin and also preservatives for blood.

- ST ammonium alkoxymethyl ionic liq antimicrobial antielectrostatic insect feeding deterrent
- IT Structure-activity relationship

(bactericidal; preparation, crystal structure, phys. and antielectrostatic properties, antimicrobial and insect feeding deterrent activity, and blood and tissue preservation ability of choline-derivative-based ionic liss.)

IT Drugs

Preservatives

(blood preservatives; preparation, crystal structure, phys. and antielectrostatic properties, antimicrobial and insect feeding deterrent activity, and blood and tissue preservation ability of choline-derivative-based ionic ligs.)

IT Molecular structure-property relationship

(elec. potential; preparation, crystal structure, phys. and antielectrostatic properties, antimicrobial and insect feeding deterrent activity, and blood and tissue preservation ability of choline-derivative-based ionic ligs.)

IT Electricity

(electrostatics; preparation, crystal structure, phys. and antielectrostatic

properties, antimicrobial and insect feeding deterrent activity, and blood and tissue preservation ability of choline-derivative-based ionic ligs.)

Structure-activity relationship

(fungicidal; preparation, crystal structure, phys. and antielectrostatic properties, antimicrobial and insect feeding deterrent activity, and blood and tissue preservation ability of choline-derivative-based ionic ligs.)

Structure-activity relationship

(insect feeding-inhibiting; preparation, crystal structure, phys. and antielectrostatic properties, antimicrobial and insect feeding deterrent activity, and blood and tissue preservation ability of choline-derivative-based ionic ligs.)

ΤТ Crystal structure

Molecular structure

(of(hydroxyethyl)dimethyl(undecyloxymethyl)ammonium chloride and of (hydroxyethyl)dimethyl(cyclododecyloxymethyl)ammonium chloride)

Antibacterial agents

Density Exchange reaction Fungicides Glass transition temperature Hydrophobicity Insect feeding inhibitors Ionic liquids Surface resistance Thermal stability

Viscosity (preparation, crystal structure, phys. and antielectrostatic properties,

antimicrobial and insect feeding deterrent activity, and blood and tissue preservation ability of choline-derivative-based ionic liqs.) Quaternary ammonium compounds, preparation

RL: AGR (Agricultural use); BSU (Biological study, unclassified); PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation, crystal structure, phys. and antielectrostatic properties, antimicrobial and insect feeding deterrent activity, and blood and tissue preservation ability of choline-derivative-based ionic ligs.)

646069-04-7P

RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (crystal structure; preparation, crystal structure, phys. and antielectrostatic properties, antimicrobial and insect feeding deterrent activity, and blood and tissue preservation ability of

choline-derivative-based ionic ligs.) 954115-51-6P 954115-52-7P 954115-53-8P 954115-54-9P 954115-55-0P 954115-63-0P 954115-64-1P 954115-65-2P 954115-66-3P 954115-67-4P

RL: AGR (Agricultural use); BSU (Biological study, unclassified); PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation, crystal structure, phys. and antielectrostatic properties, antimicrobial and insect feeding deterrent activity, and blood and tissue preservation ability of choline-derivative-based ionic ligs.)

952728-57-3P 954115-45-8P 954115-46-9P 954115-47-0P 954115-48-1P 954115-50-5P 954115-59-4P 954115-60-7P 954115-49-2P 954115-58-3P 954115-61-8P 954115-62-9P

RL: AGR (Agricultural use); BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation, crystal structure, phys. and antielectrostatic properties, antimicrobial and insect feeding deterrent activity, and blood and tissue preservation ability of choline-derivative-based ionic liqs.)

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954115-57-2P 954115-71-0P
RL: AGR (Agricultural use); BSU (Biological study, unclassified); SPN
(Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES
(Uses)
   (preparation, crystal structure, phys. and antielectrostatic properties,
   antimicrobial and insect feeding deterrent activity, and blood and
   tissue preservation ability of choline-derivative-based ionic ligs.)
954115-56-1P
RL: BSU (Biological study, unclassified); PAC (Pharmacological activity);
SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
   (preparation, crystal structure, phys. and antielectrostatic properties,
   antimicrobial and insect feeding deterrent activity, and blood and
   tissue preservation ability of choline-derivative-based ionic ligs.)
954115-69-6P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL
(Biological study); PREP (Preparation)
   (preparation, crystal structure, phys. and antielectrostatic properties,
   antimicrobial and insect feeding deterrent activity, and blood and
   tissue preservation ability of choline-derivative-based ionic ligs.)
38954-45-9P 38954-46-0P 38954-47-1P 38954-48-2P 38954-49-3P
              646068-99-7P 646069-00-3P
                                           646069-01-4P
646068-98-6P
                                                           646069-02-5P
767320-70-7P
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP
```

(Preparation); RACT (Reactant or reagent) (preparation, crystal structure, phys. and antielectrostatic properties, antimicrobial and insect feeding deterrent activity, and blood and tissue preservation ability of choline-derivative-based ionic ligs.)

IT 954115-73-2P 954115-75-4P 954115-77-6F 954115-79-8P 954115-81-2P 954115-81-2P 954115-81-2P 954115-81-2P 954115-99-2P 954115-99-2P 954115-99-2P 954115-99-2P 954116-00-8P 954116-01-9P 954116-07-5P 954116-03-1P 954116-04-2P 954116-05-3P 954116-04P 954116-07-5P RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)

(preparation, crystal structure, phys. and antielectrostatic properties, antimicrobial and insect feeding deterrent activity, and blood and tissue preservation ability of choline-derivative-based ionic liqs.)

108-01-0, N,N-Dimethylethanolamine 2351-69-1 3188-13-4, Ethoxymethyl chloride 3587-57-3 13497-61-5 13497-62-6 24566-90-3 24566-91-4 24566-92-5 24566-93-6 39979-92-5 49791-06-2 55589-62-3 58567-10-5 90076-65-6, Lithium triflimide 767320-71-8 767320-76-3 767320-78-5 767320-79-6 767320-77-4 767320-80-9 767320-81-0 767320-82-1 767320-83-2 767320-84-3 767320-85-4 954116-08-6 954116-09-7 954116-10-0 954116-11-1 954116-12-2 954116-13-3 954116-14-4 954116-15-5 954116-16-6 954116-17-7 954116-18-8 954116-19-9 954116-20-2 954116-21-3 RL: RCT (Reactant); RACT (Reactant or reagent) (preparation, crystal structure, phys. and antielectrostatic properties, antimicrobial and insect feeding deterrent activity, and blood and tissue preservation ability of choline-derivative-based ionic ligs.) 39031-08-8P IΤ

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation, crystal structure, phys. and antielectrostatic properties, antimicrobial and insect feeding deterrent activity, and blood and tissue preservation ability of choline-derivative-based ionic liqs.)

IT 954115-95-8P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation, crystal structure, phys. and antielectrostatic properties, antimicrobial and insect feeding deterrent activity, and blood and tissue preservation ability of choline-derivative-based ionic liqs.)

RE.CNT 37 THERE ARE 37 CITED REFERENCES AVAILABLE FOR THIS RECORD

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- L28 ANSWER 11 OF 21 CAPLUS COPYRIGHT 2009 ACS on STN
- AN 2007:809089 CAPLUS
- DN 148:561452
- ED Entered STN: 25 Jul 2007
- Synthesis of multi-hydroxyl and sulfonyl dual-functionalized room TT temperature ionic liquids
- AU Zhu, Guo Yang; Wang, Rong; Liu, Guo Hua; Xu, Li Oun; Zhang, Bei; Wu, Xia
- CS College of Life and Environment Science, Shanghai Normal University, Shanghai, 200234, Peop. Rep. China
- SO Chinese Chemical Letters (2007), 18(6), 633-635 CODEN: CCLEE7; ISSN: 1001-8417
- PR Chinese Chemical Society
- DT Journal
- LA English
- CC 23-12 (Aliphatic Compounds)
- OS CASREACT 148:561452
- AB Starting from the hydroxylamine (di-Me amino ethanol, triethanolamine) and 1,3-propane sultone, a series of hydroxyl and sulfonyl dual-functionalized zwitterionic salts and corresponding acidic room temperature ionic liqs. were synthesized. The hydroxyl groups of the synthesized substances were

confirmed by the 1H NMR measurement. These zwitterionic salts and ionic ligs. may be used for synthesizing other functionalized ionic ligs. or ionic liquid-polymer (polyelectrolyte).

hydroxylamine reaction propane sultone sulfonic acid; ionic liq hydroxyl sulfonyl dual functionalized toom temp prepn

Ionic liquids

NMR (nuclear magnetic resonance)

(preparation of multi-hydroxyl and sulfonyl dual-functionalized room temperature

ionic ligs, from hydroxylamine, 1,3-propane sultone, and sulfonic acids)

Sulfonic acids, reactions

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of multi-hydroxyl and sulfonyl dual-functionalized room temperature

ionic liqs. from hydroxylamine, 1,3-propane sultone, and sulfonic acids)

1026018-24-5P

RL: SPN (Synthetic preparation); PREP (Preparation)

(H-NMR spectra; preparation of multi-hydroxyl and sulfonyl dual-functionalized room temperature ionic ligs. from hydroxylamine,

1,3-propage sultone, and sulfonic acids) 75-75-2, Methanesulfonic acid 102-71-6, Triethanolamine, reactions 104-15-4, p-Toluenesulfonic acid, reactions 108-01-0, Dimethyl 1120-71-4, 1,3-Propane sultone aminoet.hanol 1493-13-6.

Trifluoromethanesulfonic acid

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of multi-hydroxyl and sulfonyl dual-functionalized room temperature

ionic liqs. from hydroxylamine, 1,3-propane sultone, and sulfonic acids)

186693-98-1P 956699-85-7P 956699-86-8P 956699-87-9P 1026018-22-3P 1026018-25-6P 1026018-26-7P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of multi-hydroxyl and sulfonyl dual-functionalized room temperature ionic liqs. from hydroxylamine, 1,3-propane sultone, and sulfonic

acids) RE.CNT 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD

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- L28 ANSWER 12 OF 21 CAPLUS COPYRIGHT 2009 ACS on STN
- AN 2007:619447 CAPLUS
- DN 147:33228
- ED Entered STN: 08 Jun 2007
- Use of hydroxylammonium salts as ionic liquid solvents for enzyme-catalyzed reactions

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IN Walker, Adam John
PA
    Bionigs Limited, UK
SO
    PCT Int. Appl., 38pp.
    CODEN: PIXXD2
DT
    Patent
LA
    English
    45-5 (Industrial Organic Chemicals, Leather, Fats, and Waxes)
    Section cross-reference(s): 23
FAN.CNT 1
    PATENT NO.
                      KIND DATE
                                       APPLICATION NO.
                                        -----
                       A1 20070607 WO 2006-GB4503
    WO 2007063327
        W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH,
            CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,
            GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN,
            KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK,
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                            20071107
                                       GB 2006-24157
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    GB 2437726
PRAT GB 2005-24700
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                              20051203
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                ECLA
                     C07C239/10; C07C239/12
OS
    MARPAT 147:33228
    An ionic liquid comprises cations of the formula R1R2R3N+-OR4, where R1, R2,
AB
    R3 and R4 are each independently selected from hydrogen and hydrocarbyl,
    the ionic liquid containing ≤ 1% of water. The ionic liqs. may be used
    as solvents for chemical or biochem. reactions, in particular, for
    enzyme-catalyzed reactions. Thus, N,N-diethylhydroxylammonium acetate
    (m.p. < -20°, viscosity 12 cP at 25°, refractive index
```

acid (60.06 g) sep. in ethanol (250 mL each), and adding the acid solution dropwise to the amine solution over 1 h, while cooling with ice and stirring. bydroxylammonium salt ionic liq solvent enzyme catalyzed reaction

(organic; use of hydroxylammonium salts as ionic liquid solvents for enzyme-catalyzed reactions)

1.414) was prepared by dissolving N,N-diethylhydroxylamine (90) and acetic

Solvents (organic; enzyme-cata Ionic liquids

ΙT

(use of hydroxylammonium salts as ionic liquid solvents for enzyme-catalyzed reactions)

T Enzymes, uses

```
RL: CAT (Catalyst use); USES (Uses)
        (use of hydroxylammonium salts as ionic liquid solvents for
        enzyme-catalyzed reactions)
     Quaternary ammonium compounds, preparation
     RL: IMF (Industrial manufacture): NUU (Other use, unclassified): PREP
     (Preparation): USES (Uses)
        (use of hydroxylammonium salts as ionic liquid solvents for
        enzyme-catalyzed reactions)
     39004-71-2P, N,N-Diethvlhvdroxvlammonium acetate
                                                      939384-89-1P
     939384-90-4P
                   939384-91-5P
                                 939384-93-7P 939384-94-8P
     939384-97-1P
     RL: IMF (Industrial manufacture); NUU (Other use, unclassified); PREP
     (Preparation); USES (Uses)
        (use of hydroxylammonium salts as ionic liquid solvents for
        enzyme-catalyzed reactions)
     939384-92-6P
     RL: IMF (Industrial manufacture); NUU (Other use, unclassified); RCT
     (Reactant); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
        (use of hydroxylammonium salts as ionic liquid solvents for
        enzyme-catalyzed reactions)
                                      75-75-2, Methanesulfonic acid 79-14-1,
     64-19-7, Acetic acid, reactions
     Glycolic acid, reactions 108-01-0, N.N-Dimethylethanolamine
     121-44-8, Triethylamine, reactions 127-09-3, Sodium acetate
     Triflic acid 3710-84-7, N,N-Diethylhydroxylamine 7647-01-0,
     Hydrochloric acid, reactions 7722-84-1, Hydrogen peroxide, reactions
     82113-65-3, Bis(trifluoromethylsulfonyl)imide
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (use of hydroxylammonium salts as ionic liquid solvents for
        enzyme-catalyzed reactions)
RE.CNT 19
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RE
(1) Anon
(2) Anon
(3) Anon
(4) Anon
(5) Anon
(6) Anon
(7) Anon
(8) Anon; GAZZ CHIM ITAL 1954, V84, P915
(9) Anon; J AM CHEM SOC 1927, V49, P1539
(10) Anon; J AM CHEM SOC 1947, V69, P1731
(11) Anon; J CHIN CHEM SOC 1977, V24, P115
(12) Anon; J MOL STRUCT 1990, V239, P1
(13) Anon; JUSTUS LIEBIGS ANN CHEM 1913, V397, P275
(14) Anon; YAKUGAKU ZASSHI 1940, V60, P24
(15) Hecht Stacie E; US 2006094616 A1 2006
(16) Nippon Telegraph & Telephone; JP 2005149982 A 2005 CAPLUS
(17) Takami, N; JP 11086905 A 1999 CAPLUS
(18) Umemoto Teruo: US 2006094882 A1 2006
(19) Wehner Wolfgang; US 4578489 A 1986 CAPLUS
L28 ANSWER 13 OF 21 CAPLUS COPYRIGHT 2009 ACS on STN
AN
     2007:433670 CAPLUS
DN
     146:448426
    Entered STN: 19 Apr 2007
    Multi-functional ionic liquid compositions for
     overcoming polymorphism and imparting improved properties for active
     ingredients
    Rogers, Robin D.; Daly, Daniel T.; Swatloski, Richard P.; Hough, Whitney
    L.; Davis, James Hillard; Smiglak, Marcin; Pernak, Juliusz; Spear, Scott
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PA

The University of Alabama, USA

SO PCT Int. Appl., 199pp.

CODEN: PIXXD2

DT Patent

LA English

CC 63-6 (Pharmaceuticals)

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	RW:	AT, BE, IS, IT, CF, CG, GM, KE, KG, KZ,	BG, C LT, I CI, C LS, N	CH, CY LU, LV CM, GA AW, MZ	, CZ, , MC, , GN, , NA,	DE, NL, GQ, SD,	DK, PL, GW, SL,	EE, PT, ML, SZ,	RO, MR, TZ,	SE, NE,	SI, SN,	SK, TD,	TR, TG,	BF, BW,	BJ, GH,
	AU 20063 CA 26250 US 20070 EP 1931			A1 A2	2007 2007 2008	0419 0426 0618			006- 006- 006-	2625 5459 8362	004 38 36		2 2 2		010 010 010
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EP	1931760	NCL IPC IPC	I C1	14/184 11D001 11D001	7-00	[I,A]					0			
KR IN	200800461 20080686 2008DN03 101326275	79 IPC 782 IPC	I CI	11D001 11D001	7-00 7-00	[I,A [ICM] ,7]								
AB	Disclose			ligs.				f pr	epar	ing	ioni	c li	quid	com	pns.

AB Disclosed are ionic ligs. and methods of preparing ionic liquid compns. of active pharmaceutical, biol., nutritional, and energetic ingredients. Also disclosed are methods of using the compns. described herein to overcome polymorphism, overcome solubility and delivery problems, to control release rates, add functionality, enhance efficacy (synergy), and improve ease of use and manufacture Hexadecylpyridinium valproic acid was prepared by

the reaction of hexadecylpyridinium chloride with sodium valproate.

pharmaceutical ionic liq multifunctional property

IT Quaternary ammonium compounds, reactions

RL: RCT (Reactant); RACT (Reactant or reagent)

(alkylbenzyldimethyl, chlorides; multifunctional ionic liquid compns. for overcoming polymorphism and imparting improved properties for active ingredients)

IT Analgesics

Anesthetics
Anti-inflammatory agents
Anti-bacterial agents
Antiviral agents
Crystal polymorphism
Dietary supplements
Drug delivery systems
Dyes
Food additives

Herbicides Ionic liquids

Metathesis Neutralization

Nutrition, animal Pesticides

Preservatives Solvents

Sunscreens Surfactants

Thickening agents Viscosity

(multifunctional ionic liquid compns. for overcoming polymorphism and imparting improved properties for active ingredients)

IT Growth regulators, plant

RL: AGR (Agricultural use); BIOL (Biological study); USES (Uses) (multifunctional ionic liquid compns. for overcoming polymorphism and imparting improved properties for active ingredients)

63-36-5DP, benzalkonium salts, biological studies 137-58-6DP, Lidocaine, complex with silver 766-76-7DP, benzalkonium salts, biological studies 7428-34-4P 16766-82-8DP, benzalkonium salts and ternary salts with acesulfamate or sulfathiazolate 17263-38-6DP, benzalkonium salts, biological studies 27059-75-2P 28598-04-1P 45297-26-5DP, benzalkonium salts and ternary salts with mepenzolate 46480-62-0DP. benzalkonium salts and ternary salts with saccharinate 54836-26-9DP, benzalkonium salts 56965-02-7DP, benzalkonium derivs. 71303-05-4DP, benzalkonium salts 112210-22-7P 119441-67-7DP, benzalkonium salts and ternary salts with saccharinate 132781-87-4P 136869-01-7DP, benzalkonium salts 479620-35-4P 736071-66-2DP, benzalkonium salts 934544-24-8P 934544-25-9P 934544-26-0P 934544-27-1P 934544-28-2P 934544-29-3P 934544-30-6P 934544-31-7P 934544-32-8DP, benzalkonium salts 934544-33-9P 934544-34-0P 934544-35-1DP, benzalkonium salts 934544-36-2P 934544-37-3P 934544-38-4P 934544-39-5P 934544-40-8P 934544-41-9P 934544-42-0P 934544-43-1P, biological studies 934544-44-2P 934544-46-4P 934544-47-5P 934544-48-6P 934544-50-0P 934544-52-2P 934544-54-4P 934544-55-5P 934544-49-7P 934544-56-6P 934544-61-3P 934544-62-4P 934544-63-5P 934544-64-6P 934544-65-7P 934544-66-8P 934544-67-9P 934544-72-6P 934544-73-7P 934544-75-9P 934544-86-2P 934544-97-3P 934544-80-8P 93454-83-PP 934544-86-2P 934544-87-3P 934544-97-3P 934544-90-8P 934544-92-0P 934545-93-P9 934545-09-2P 934545-16-1P 934545-19-4P 934545-23-0P 934545-25-2P 934545-27-4P 934545-29-6P 934545-31-0P 934545-33-2P 934545-34-3P 934545-36-5P 934545-38-7P 934545-41-2P 934545-43-4P

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     RL: PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use);
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        (multifunctional ionic liquid compns. for overcoming polymorphism and
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     50-78-2 54-21-7 54-64-8 59-67-6, 3-Pvridinecarboxvlic acid,
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     Hexadecylpyridinium chloride 127-56-0 128-44-9 140-10-3, reactions
     144-74-1 532-32-1 577-11-7, Sodium docusate 582-25-2, Potassium
     benzoate 1069-66-5 1421-89-2, 2-(Dimethylamino)ethyl acetate
     2353-45-9 2390-68-3 3006-15-3, Colawet MA 80 6484-89-5 7173-51-5
     7761-88-8, Nitric acid silver(1+) salt (1:1), reactions 13497-61-5,
     Chloromethyl dodecyl ether 15307-79-6 15687-27-1 24566-93-6, Chloromethyl undecyl ether 26159-34-2, Sodium napropotassium 59703-84-3
     61334-06-3, Acesulfame sodium 66357-59-3, Ranitidine hydrochloride
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L28 ANSWER 14 OF 21 CAPLUS COPYRIGHT 2009 ACS on STN
    2006:681182 CAPLUS
    145:145001
    Entered STN: 14 Jul 2006
    Preparation of quaternary ammonium compounds as base stable ionic
     Earle, Martyn John; Frohlich, Ute; Hug, Susanne; Katdare, Suhas; Lukasik,
     Rafal Marcin; Bogel, Ewa; Plechkova, Natalia Vladimirovna; Seddon, Kenneth
     Richard
     The Oueen's University of Belfast, UK
SO PCT Int. Appl., 35 pp.
    CODEN: PIXXD2
    Pat.ent.
   English
     ICM B01J
     21-2 (General Organic Chemistry)
FAN.CNT 1
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VN, YU, ZA, ZM, ZW

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EP 1841533
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L01J; L01J; L01J; L01J; L01J; L01J; L01J; L01J; L01J; M07C; M07C; M07D; M07D JP 2008526822 TPCT C07B0061-00 [I,A]; C07C0221-00 [I,A]; C07C0225-12 [I,A]; C07C0225-00 [I,C*]; C07C0049-623 [I,A]; C07C0049-203 [I,A]; C07C0049-403 [I,A]; C07C0045-72 [I,A]; C07C0049-603 [I,A]; C07C0049-00 [I,C*]; C07C0045-74 [I,A]; C07C0045-00 [I,C*]; C07C0211-63 [N,A]; C07C0211-00 [N,C*]; C07C0215-08 [N,A]; C07C0215-00 [N,C*]; C07F0009-54 [N,A]; C07F0009-00 IN,C*1 FTERM 4H006/AA02; 4H006/AA03; 4H006/AB83; 4H006/AC13; 4H006/AC21; 4H006/AC22; 4H006/AC28; 4H006/AC52; 4H006/AD40; 4H050/AA03; 4H050/AB83 MX 2007008160 IPCI B01J0031-02 [I,C]; C07C0209-60 [I,A]; C07C0209-00 [I,C*]; C07C0045-74 [I,A]; C07C0045-00 [I,C*] KR 2007101301 IPCI B01J0031-02 [I,A]; C07C0313-00 [I,A]; C07C0045-66 [I,A]; C07C0045-00 [I,C*] CN 101137436 IPCI B01J0031-02 [I,A]; C07C0209-60 [I,A]; C07C0209-00 [I,C*]; C07C0045-74 [I,A]; C07C0045-00 [I,C*]

OS MARPAT 145:145001

AB The present invention relates to novel base stable ionic liqs. such as N-alkyl-N,N-dimethylethanolamine salts, N-alkyl-DABCO salts, N-alkyl-tetramethylenediamine salts, and N-alkyl-M-methylpyrazolium salts and uses thereof as solvents in chemical reactions, especially base catalyzed

chemical reactions and reactions comprising the use of strong bases. Chemical reactions include Mannich reaction, Robinson annulation, Michael reaction,

Heck reaction, epoxidn., hydrogenation, aldol condensation, transesterification, esterification, hydrolysis, oxidation, reduction,

hydration,

dehydration, substitution, aromatic substitution, addition (including to carbonyl groups), elimination, polymerization, depolymm., oligomerization, dimerization, coupling, electrocyclisation, isomerization, carbene formation, epimerization, inversion, rearrangement, photochem. microwave assisted, thermal, sonochem, and disproportionation reactions. Thus, N-alkylation of 2-(dimethylamino)ethanol by Pr loddde and treatment of the resulting N-(2-hydroxyethyl)-N,N-dimethyl-N-propylammonium iodide with LiNTi2 (If = CT3502) gave Prhe2N+CH2CH2OH.(NTI2)-. Cyclopentanone was condensed with pentanal in the presence of L-propine catalyst in ELMe2N+CH2CH2OH.(NTI2)- at room temperature for 18 h to give 94% 2-pentyl-2-cyclopenten-l-one.

ST aldol condensation quaternary ammonium compd solvent prepn; quaternary ammonium compd prepn solvent base stable ionic liq; Mannich reaction Robinson annulation Michael reaction solvent ionic liq; alkyldimethylethanolamine salt prepn solvent base stable ionic liq; alkyl DABCO salt prepn solvent base stable ionic liq; alkyltetramethylenediamine salt prepn solvent base stable ionic liq; alkyltetramethylenediamine solvent base stable ionic liq; alkylmethylpyrazolium salt prepn solvent base stable ionic liq;

IT Arviation

(Heck; preparation of quaternary ammonium compds. as base stable ionic liqs. as solvents in base-catalyzed chemical reactions)

IT Cyclization

(Robinson annulation; preparation of quaternary ammonium compds. as base stable ionic liqs. as solvents in base-catalyzed chemical reactions) Substitution reaction

(aromatic; preparation of quaternary ammonium compds. as base stable ionic liqs. as solvents in base-catalyzed chemical reactions)

IT Cvclization

(electrocyclic; preparation of quaternary ammonium compds. as base stable ionic liqs. as solvents in base-catalyzed chemical reactions)

Carbenes (methylene derivatives)

RL: SPN (Synthetic preparation); PREP (Preparation)

```
(formation; preparation of quaternary ammonium compds. as base stable ionic
        ligs. as solvents in base-catalyzed chemical reactions)
    Substitution reaction, nucleophilic
        (inversion reaction; preparation of quaternary ammonium compds. as base
       stable ionic ligs, as solvents in base-catalyzed chemical reactions)
    Microwave
        (microwave assisted reactions; preparation of quaternary ammonium compds. as
       base stable ionic ligs. as solvents in base-catalyzed chemical reactions)
    Polymerization
        (oligomerization; preparation of quaternary ammonium compds. as base stable
       ionic liqs. as solvents in base-catalyzed chemical reactions)
    Solvents
        (organic; preparation of quaternary ammonium compds. as base stable ionic
ligs.
       as solvents in base-catalyzed chemical reactions)
ΤТ
    Addition reaction
    Aldol condensation
    Autoxidation
    Coupling reaction
    Dehydration reaction
    Depolymerization
    Dimerization
    Disproportionation
    Elimination reaction
    Epoxidation
    Hydration, chemical
    Hydrogenation
    Hydrolysis
      Ionic liquids
    Isomerization
    Mannich reaction
    Michael reaction
    Photolysis
    Polymerization
    Rearrangement
    Reduction
    Substitution reaction
    Transesterification
        (preparation of quaternary ammonium compds. as base stable ionic liqs. as
       solvents in base-catalyzed chemical reactions)
    Quaternary ammonium compounds, preparation
    RL: NUU (Other use, unclassified); SPN (Synthetic preparation); PREP
     (Preparation); USES (Uses)
        (preparation of quaternary ammonium compds. as base stable ionic liqs. as
       solvents in base-catalyzed chemical reactions)
    Reaction
       (sonochem. reactions; preparation of quaternary ammonium compds. as base
       stable ionic ligs, as solvents in base-catalyzed chemical reactions)
    Reaction
        (thermal; preparation of quaternary ammonium compds. as base stable ionic
        ligs. as solvents in base-catalyzed chemical reactions)
    78-59-1 123-42-2
                         141-79-7 504-20-1
                                              27203-92-5
    RL: PRPH (Prophetic)
        (Preparation of quaternary ammonium compounds as base stable
       ionic liquids)
    111-66-0P, 1-Octene
                         111-67-1P, 2-Octene 898256-56-9P,
    1,3,5-Trimethylpyrazole hydrobromide
    RL: BYP (Byproduct); PREP (Preparation)
        (preparation of quaternary ammonium compds. as base stable ionic liqs. as
       solvents in base-catalyzed chemical reactions)
    123-75-1, Pyrrolidine, uses 147-85-3, L-Proline, uses 1305-62-0,
    Calcium hydroxide, uses 1310-73-2, Sodium hydroxide, uses 4111-54-0,
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Lithium diisopropylamide 6552-73-4, Sodium methoxide-d3 7789-23-3D,
Potassium fluoride, supported on alumina 14014-06-3, Sodium hydroxide-d
20734-58-1, Proton sponge
RL: CAT (Catalyst use); USES (Uses)
   (preparation of quaternary ammonium compds. as base stable ionic liqs. as
   solvents in base-catalyzed chemical reactions)
898256-55-8P
RL: NUU (Other use, unclassified); RCT (Reactant); SPN (Synthetic
preparation); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
   (preparation of quaternary ammonium compds, as base stable ionic ligs, as
   solvents in base-catalyzed chemical reactions)
4535-70-0P, N-Ethyl-N-(2-hydroxyethyl)-N,N-dimethylammonium bromide
7009-61-2P, N-Dodecyl-N-(2-hydroxyethyl)-N, N-dimethylammonium bromide
13186-62-4P, N-(2-Hydroxyethyl)-N, N-dimethyl-N-propylammonium bromide
15061-91-3P, N-(2-Hydroxyethyl)-N,N-dimethyl-N-octadecylammonium bromide
28228-54-8P, N-(2-Hydroxyethyl)-N-hexyl-N,N-dimethylammonium chloride
28508-15-8P, N-Butyl-N-(2-hydroxyethyl)-N, N-dimethylammonium bromide
33249-14-8P 39995-55-6P, N-Decyl-N-(2-hydroxyethyl)-N, N-dimethylammonium
bromide 50938-57-3P 62634-05-3P 62634-13-3P 62634-16-6P
62634-17-7P 122135-71-1P, N-(2-Hydroxyethyl)-N, N-dimethyl-N-
octylammonium bromide 123714-89-6P,
N-Decvl-N-[2-(dimethylamino)ethyl]-N, N-dimethylammonium bromide
171874-92-3P 202256-55-1P 202256-57-3P 214349-74-3P 219787-58-3P.
N-Hexyl-N-(2-hydroxyethyl)-N, N-dimethylammonium bromide 342789-81-5P
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783354-56-3P 882509-35-4P 854102-71-9P 863031-17-8P 885456-22-4P 898256-40-1P 898256-41-2P, N-(2-Butoxyethyl)-N-octyl-N,N-dimethylammonium bromide 898256-42-3P, N-[2-(Rexyloxy)ethyl]-N-hexyl-N,N-dimethylammonium bromide 898256-43-4P, N-(2-Butoxyethyl)-N-butyl-N, N-dimethylammonium bromide 898256-44-5P, N,N-Dimethyl-N-octyl-N-[2-(octyloxy)ethyl]ammonium bromide 898256-45-6P, N,N-Decyl-N-[2-(dectyloxy)ethyl]ammonium bromide 898256-46-6P, N-Decyl-N-[2-(dectyloxy)ethyl]ammonium bromide 898256-46-6P,

trifluoromethanesulfonate 898256-48-9P,
N-(2-Hydroxyethyl)-N,N-dimethyl-N-propylammonium tetrafluoroborate
898256-49-0P, N-(2-Hydroxyethyl)-N,N-dimethyl-N-propylammonium
trifluoromethanesulfonate 898256-50-3P 898256-51-4P 898256-52-5P
898256-53-6P, N-[2-(Dimethylamino)ethyl]-N,N-dimethyl-N-pentylammonium

N-Ethyl-N-(2-hydroxyethyl)-N,N-dimethylammonium tetrafluoroborate 898256-47-8P, N-Ethyl-N-(2-hydroxyethyl)-N,N-dimethylammonium

bromide 898256-54-7P, N-12-(Dimethylamino)ethyll-N, N-dimethyl-Noctylammonium bromide 898256-57-0P 898256-59-2P 898256-60-5P 898256-61-6P 898256-62-7P 898256-38-P 898256-64-9P 898256-65-0P

898256-66-1P 898256-68-3P 898256-70-7P 898256-72-9P 898256-74-1P 898256-75-2P 898256-75-4P 898256-78-5P 898256-79-6P 898256-80-9P 898256-82-1P 898256-83-2P 898256-84-3P 898256-85-4P 898256-85-5P

RL: NUU (Other use, unclassified); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)

(preparation of quaternary ammonium compds. as base stable ionic liqs. as solvents in base-catalyzed chemical reactions)

IT 1128-08-1P, Dihydrojasmone

RL: PNU (Preparation, unclassified); PREP (Preparation) (preparation of quaternary ammonium compds. as base stable ionic liqs. as solvents in base-catalyzed chemical reactions)

T 64-17-5, Ethanol, reactions 71-23-8, n-Propanol, reactions 71-36-3, n-Butanol, reactions 71-41-0, n-Pentanol, reactions 74-96-4, Ethyl bromide 78-94-4, Methyl vinyl ketone, reactions 106-94-5, n-Propyl bromide 107-08-4, Propyl iodide 108-01-0, 2-(Dimethylamino)ethanol 108-94-1, Cyclohexanone, reactions 109-65-9, n-Butyl bromide 110-18-9, N,N,N',N'-Tetramethylethylenediamine 110-52-3, Pentynl bromide 110-62-3, Pentanal 110-91-8, Morpholine,

reactions 111-25-1, n-Hexyl bromide 111-27-3, n-Hexanol, reactions 111-83-1, n-Octyl bromide 111-87-5, n-Octanol, reactions 112-29-8,

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n-Decyl bromide 112-30-1, 1-Decanol 112-53-8, 1-Dodecanol 112-71-0,
    n-Tetradecyl bromide 112-72-1, n-Tetradecanol 112-82-3, n-Hexadecyl
              112-89-0, n-Octadecvl bromide 112-92-5, n-Octadecanol
    bromide
    120-92-3, Cyclopentanone 124-63-0, Methanesulfonyl chloride
                                                                    143-15-7.
    n-Dodecyl bromide 280-57-9, DABCO 504-02-9, 1,3-Cyclohexanedione
    544-10-5, n-Hexyl chloride 930-36-9 1072-91-9, 1,3,5-Trimethylpyrazole
    1122-58-3, 4-Dimethylaminopyridine 1193-55-1,
    2-Methylcyclohexane-1,3-dione 16940-81-1, Hexafluorophosphoric acid
    21324-39-0, Sodium hexafluorophosphate 30525-89-4, Paraformaldehyde
    36653-82-4, n-Hexadecanol 90076-65-6, Lithium
    bis(trifluoromethanesulfonimide)
    RL: RCT (Reactant); RACT (Reactant or reagent)
        (preparation of quaternary ammonium compds. as base stable ionic liqs. as
       solvents in base-catalyzed chemical reactions)
    62-50-0P, Ethyl methanesulfonate 1912-31-8P, Propyl methanesulfonate
    1912-32-9P, Butyl methanesulfonate 3240-94-6P, 2-(Morpholin-4-yl)ethyl
    chloride 5073-65-4P, 2-Methyl-2-(3-oxobutyl)cyclohexane-1,3-dione
    6222-16-8P, Tetradecyl methanesulfonate 6968-20-3P, Pentyl
    methanesulfonate 16156-50-6P, Hexyl methanesulfonate
                                                            16156-52-8P,
    Octyl methanesulfonate 16424-35-4P, 2-Pentylidenecyclopentanone
    20779-14-0P, Hexadecvl methanesulfonate
                                             26942-62-1P,
    2-(3-0xobutv1)cvclohexanone 32492-73-2P,
    N-(2-Hydroxyethyl)-N, N-dimethyl-N-propylammonium iodide
                                                             34084-81-6P.
    2-(3-Oxobutyl)cyclohexane-1,3-dione 41233-29-8P, Decyl methanesulfonate
    42558-01-0P, 2-(1-Hydroxypenty1)cyclopentanone 159438-86-5P, Undecyl
    methanesulfonate
    RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (preparation of quaternary ammonium compds. as base stable ionic liqs. as
       solvents in base-catalyzed chemical reactions)
    100-58-3, Phenylmagnesium bromide
    RL: RGT (Reagent); RACT (Reactant or reagent)
        (preparation of quaternary ammonium compds. as base stable ionic ligs. as
       solvents in base-catalyzed chemical reactions)
    1196-55-0P, 2,3,4,4a,5,6,7,8-Octahydronaphthalen-2-one
                                                             24071-91-8P,
    2-[(Morpholin-4-yl)methyl]cyclohexanone
                                             25564-22-1P.
    2-Pentyl-2-cyclopenten-1-one
                                  42576-97-6P,
    1, 2, 3, 4, 6, 7, 8, 8a-Octahydronaphthalene-1, 6-dione
                                                     99178-63-9P,
     4-[2-[2-(Dimethylamino)ethoxy]ethyl]morpholine
                                                    100348-93-4P
    RL: SPN (Synthetic preparation); PREP (Preparation)
        (preparation of quaternary ammonium compds. as base stable ionic ligs. as
       solvents in base-catalyzed chemical reactions)
RE.CNT 4
             THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD
(1) Anon; DE 10247578 A1 CAPLUS
(2) Anon; US 20040097755 A1 CAPLUS
(3) Anon; WO 2004029004 A1 CAPLUS
(4) Anon; US 6552232 B2 CAPLUS
L28 ANSWER 15 OF 21 CAPLUS COPYRIGHT 2009 ACS on STN
    2006:681152 CAPLUS
    145:145000
    Entered STN: 14 Jul 2006
    Preparation of quaternary ammonium compounds as basic ionic
    liquids
    Earle, Martyn John; Seddon, Kenneth Richard; Forsyth, Stewart; Frohlich,
    Ute; Gunaratne, Nimal; Katdare, Suhas
    The Queen's University of Belfast, UK
    PCT Int. Appl., 51 pp.
    CODEN: PIXXD2
    Patent
    English
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CN 10113743	7	A	20080305		2006-8	800056	70	20070	0822
PRAI GB 2005-29		A	20050104						
WO 2006-GB6		W	20060104						
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			5-62 [I,A						12
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			B01J0031						
			7-04 [I,A						-00
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			3-32 [I,A						
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			/02E4; B0					CU/B061	1/00;
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			/72+49/49					70043/12	-1-2/1/
			/73+49/40						
			/74+49/64					3B+	
			/54C; C07						L01J;
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EP 1853385	IPCI		1-02 [I,A		0301-	12 [].	A1; C0	7D0301-0	0
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                       4C055/CA01; 4C055/DA52; 4C055/DB02; 4C055/FA01;
                       4C055/FA37; 4C064/AA06; 4C064/CC02; 4C064/DD01;
                       4C064/EE01; 4C064/FF03; 4C064/GG01; 4C064/HH04;
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                       4C069/CC13; 4H006/AA01; 4H006/AA03; 4H006/AB40;
                       4H006/AB80; 4H006/AC11; 4H006/AC25; 4H006/AC28;
                       4H006/AC41; 4H006/BB19; 4H006/BB24; 4H006/BJ20;
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                       4H006/BR70; 4H006/BU50; 4H039/CA19; 4H039/CA40;
                       4H039/CA41; 4H039/CA42; 4H039/CE90; 4H039/CF30;
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KR 2007104899
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CN 101137437
                IPCI
                      B01J0031-02 [I,A]; C07D0301-12 [I,A]; C07D0301-00
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[I,C*]; C07C0209-60 [I,A]; C07C0209-00 [I,C*]; C07C0045-72 [I,A]; C07C0045-69 [I,A]; C07C0045-62

[I,A]; C07C0045-00 [I,C*]; C07B0037-04 [I,A]; C07B0037-00 [I,C*]

OS CASREACT 145:145000; MARPAT 145:145000

AB This invention relates to preparation and use of ionic liqs. as solvents in base-catalyzed chemical reactions wherein the ionic liquid is composed of at least one species of cation and at least one species of anion, characterized in that a cation of the ionic liquid comprises a pos. charge molety and a basic moiety, and further wherein such ionic liqs. may be used as promoters or catalysts for the chemical reactions. Chemical reactions include Heck Reaction, Suzuki coupling, nucleophilic displacement reactions, hydrolysis, esterification, transesterification, aldol reactions, epoxidn. hydrogenation, condensation, oxidation reduction,

hydration,

dehydration, substitution, aromatic substitution, addition (including to carbonyl groups), elimination, polymerization, depolymn., oligomerization, dimerization, coupling, electrocyclic, isomerization, carbene formation, epimerization, inversion, rearrangement, photochem., microwave assisted, thermal, sonochem. and disproportionation reactions. Thus, etherification of 2-(dimethylamino)ethanol with 2-(disopropylamino)ethanol hydrochloride followed by regioselective quaternization with Et bromide and treatment with lithium bis(trifilmide) gave a room temperature ionic liquid of formula PrNMe2N+CH2CH2OCH2CH2N(i-Fr)2.N-(SOCF3)2 (I). Bpoxidn. of chalcone in this ionic liquid I gave chalcone epoxide with 100% conversion.

quaternary ammonium compd prepn solvent catalyst ionic liq

IT Arylation

(Heck; preparation of quaternary ammonium compds. as basic ionic liqs. in base-catalyzed chemical reactions)

IT Substitution reaction (aromatic; preparation of quaternary ammonium compds. as basic ionic ligs.

base-catalyzed chemical reactions)

IT Cyclization

(electrocyclic; preparation of quaternary ammonium compds. as basic ionic ligs. in base-catalyzed chemical reactions)

IT Carbenes (methylene derivatives)

RL: SPN (Synthetic preparation); PREP (Preparation)

(formation; preparation of quaternary ammonium compds. as basic ionic liqs. in base-catalyzed chemical reactions)

TT Dec-ti-e

(inversion; preparation of quaternary ammonium compds. as basic ionic liqs. in base-catalyzed chemical reactions)

IT Reaction

(microwave-assisted; preparation of quaternary ammonium compds. as basic ionic ligs. in base-catalyzed chemical reactions)

IT Polymerization

(oligomerization; preparation of quaternary ammonium compds. as basic ionic liqs. in base-catalyzed chemical reactions)

IT Addition reaction
Aldol condensation

Condensation reaction Coupling reaction

Dehydration reaction Depolymerization

Dimerization

Dimerization Disproportionation

Elimination reaction

Epimerization Epoxidation

Hydration, chemical

Hydrogenation

Hydrolysis

Ionic liquids

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Photolysis
Polymerization
Rearrangement
Reduction
Substitution reaction
Substitution reaction, nucleophilic
Suzuki coupling reaction
Transesterification
   (preparation of quaternary ammonium compds. as basic ionic liqs. in
   base-catalyzed chemical reactions)
Quaternary ammonium compounds, uses
RL: CAT (Catalyst use); NUU (Other use, unclassified); USES (Uses)
   (preparation of quaternary ammonium compds. as basic ionic liqs. in
   base-catalyzed chemical reactions)
Reaction
   (sonochem.; preparation of quaternary ammonium compds. as basic ionic ligs.
   in base-catalyzed chemical reactions)
Reaction
   (thermal; preparation of quaternary ammonium compds. as basic ionic ligs. in
   base-catalyzed chemical reactions)
78-59-1 123-42-2 141-79-7 504-20-1
                                           15409-60-6 67382-39-2
123134-25-8
RL: PRPH (Prophetic)
   (Preparation of quaternary ammonium compounds as basic ionic
   liquids)
147-85-3, L-Proline, uses 3375-31-3
RL: CAT (Catalyst use); USES (Uses)
   (preparation of quaternary ammonium compds. as basic ionic ligs. in
   base-catalyzed chemical reactions)
898535-34-7P
RL: CAT (Catalyst use); NUU (Other use, unclassified); RCT (Reactant); SPN
(Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent);
USES (Uses)
   (preparation of quaternary ammonium compds. as basic ionic liqs. in
   base-catalyzed chemical reactions)
33249-14-8P
             50938-57-3P 62634-05-3P
                                         62634-13-3P 62634-16-6P
62634-17-7P
             106303-35-9P
                            114203-57-5P,
4-(Dimethylamino)-1-ethylpyridinium bromide
                                            123714-89-6P 171874-92-3P
171894-19-2P, N-[2-(Dimethylamino)ethyll-N, N-dimethyl-N-octadecylammonium
bromide 202256-55-1P 202256-57-3P 214349-74-3P 289910-39-0P.
N-Ethyl-N-[2-(dimethylamino)ethyl]-N, N-dimethylammonium bromide
395677-61-9P, 4-(Dimethylamino)-1-hexylpyridinium bromide
                                                            783354-56-3P
863031-17-8P
             898256-51-4P
                             898256-52-5P
                                            898256-53-6P,
N-[2-(Dimethylamino)ethyl]-N, N-dimethyl-N-pentylammonium bromide
898256-54-7P, N-[2-(Dimethylamino)ethyl]-N, N-dimethyl-N-octylammonium
         898256-84-3P, 4-(Dimethylamino)-1-ethylpyridinium
bromide
                                  898535-32-5P
methanesulfonate 898256-85-4P
                                                 898535-36-9P
898535-38-1P 898535-40-5P 898535-42-7P 898535-44-9P
                                                           898535-44-9P
              898535-49-4P 898535-51-8P
898535-47-2P
                                            898535-53-0P
RL: CAT (Catalyst use); NUU (Other use, unclassified); SPN (Synthetic
preparation); PREP (Preparation); USES (Uses)
   (preparation of quaternary ammonium compds. as basic ionic liqs. in
   base-catalyzed chemical reactions)
62-50-0, Ethyl methanesulfonate 74-96-4, Ethyl bromide 75-03-6, Ethyl
iodide 78-94-4, Vinyl methyl ketone, reactions 94-41-7, Charcone 96-79-7, 2-(Diisopropylamino)ethyl chloride 100-52-7, Benzaldehydd
reactions 105-56-6, Ethyl cyanoacetate 106-94-5, n-Propyl bromide
108-01-0, N,N-Dimethylethanolamine 109-65-9, n-Butyl bromide
110-18-9, N,N,N',N'-Tetramethylethylenediamine 110-53-2, n-Pentyl
bromide 110-62-3, Pentanal 111-18-2 111-25-1, n-Hexyl bromide
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Isomerization Oxidation

IT

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111-83-1, n-Octyl bromide 112-29-8, n-Decyl bromide 112-71-0,
    n-Tetradecyl bromide 112-82-3, n-Hexadecyl bromide 112-89-0,
    n-Octadecyl bromide 120-92-3, Cyclopentanone 120-94-5,
     1-Methylpyrrolidine 143-15-7, n-Dodecyl bromide 280-57-9, DABCO
     504-02-9, 1,3-Cyclohexanedione 513-42-8, 2-Methyl-2-propenol 542-69-8,
     n-Butyl iodide 598-56-1, N-Ethyldimethylamine 616-47-7,
     1-Methyl-1H-imidazole 1122-58-3, 4-Dimethylaminopyridine
                                                               1193-55-1.
     2-Methylcyclohexane-1,3-dione 1704-62-7,
     2-[2-(Dimethylamino)ethoxylethanol 3647-69-6,
     1-(Morpholin-4-v1)-2-chloroethane hydrochloride 4261-68-1,
     2-(Diisopropylamino)ethyl chloride hydrochloride 5073-65-4,
     2-Methyl-2-(3-oxobutyl)cyclohexane-1,3-dione 13586-68-0 16156-50-6,
     Hexyl methanesulfonate 35779-04-5, 4-tert-Butyl-1-iodobenzene
     90076-65-6, Lithium bis(trifluoromethanesulfonimide)
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (preparation of quaternary ammonium compds. as basic ionic liqs. in
        base-catalyzed chemical reactions)
     16424-35-4P, 2-Pentylidenecyclopentanone 25564-22-1P,
     2-Pentyl-2-cyclopenten-1-one 34084-81-6P,
     2-(3-0xobutyl)cyclohexane-1,3-dione 42558-01-0P,
     2-(1-Hydroxypentyl)cyclopentanone 99178-63-9P,
     4-[2-[2-(Dimethylamino)ethoxylethyl]morpholine
                                                    898535-33-6P,
     N, N-Diisopropyl-N-[2-[2-(dimethylamino)ethoxylethyllamine 898535-45-0P
     959467-54-0P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (preparation of quaternary ammonium compds. as basic ionic ligs. in
        base-catalyzed chemical reactions)
     80-54-6P, β-Lilial 2169-69-9P, Ethyl
     (E)-2-benzylidene-2-cyanoacetate 5411-12-1P, Chalcone epoxide
     14533-87-0P, Ethyl (Z)-2-benzylidene-2-cyanoacetate 42576-97-6P
     100348-93-4P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (preparation of quaternary ammonium compds. as basic ionic ligs. in
        base-catalyzed chemical reactions)
RE.CNT 5
            THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD
(1) Anon; DE 10247578 A1 CAPLUS
(2) Anon; US 20020035297 A1 CAPLUS
(3) Anon; US 20040097755 A1 CAPLUS
(4) Anon; WO 2004029004 A1 CAPLUS
(5) Anon; WO 2005019185 A1 CAPLUS
L28 ANSWER 16 OF 21 CAPLUS COPYRIGHT 2009 ACS on STN
AN
    2005:1090138 CAPLUS
DN
   143:386681
   Entered STN: 12 Oct 2005
    Ionic liquids containing protonated primary, secondary
    or tertiary ammonium ions
    Walker, Adam John
    The University of York, UK
    Brit. UK Pat. Appl., 62 pp.
    CODEN: BAXXDU
    Patent
    English
    ICM C07C215-08
     ICS C07C215-12; C07C217-30
     23-4 (Aliphatic Compounds)
     Section cross-reference(s): 45
FAN.CNT 1
    PATENT NO.
                       KIND DATE
                                      APPLICATION NO. DATE
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	WO	2005097 2005097			A2 A3		2005 2005	1020			005-					0050			
		W: AE	, AG,		AM,	AT,	AU,	AZ,											
		GE	, GH,	GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	KE,	KG,	KM,	KP,	KR,	KZ,		
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		RW: BW	, GH, , BY,																
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CLAS		2005-GB	1364		W		2005	0407											
	TENT NO. CLASS				PATE														
GB	241	2912	ICM ICS		C07C			0070	217	20									
			IPC		C07C215-12; C07C217-30 C07C0215-00 [I,C]; C07C0215-08 [I,A]; C07C0215-12														
			IPC	R	[I,A]; C07C0217-00 [I,C]; C07C0217-30 [I,A] C07C0215-00 [I,C]; C07C0215-08 [I,A]; C07C0215-12														
							; C07C0215-40 [I,A]; C07C0217-00 [I,C]; 217-30 [I,A]												
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					C07C	0217	-30	[I,A]										
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			IPC	R	[I,A C07C							40 f	T.A1	. B0	1.100	31-0	2		
				• `	[I,C]; B	01J0	031-	02 [I,A]	; B0	1J00	31-0	4 [I	,C];				
					B01J]; C	07C0	217-] 00	I,C*]; C	07C0	217-	30 [I,A]		۷		
WO	200	5097731	ECL IPC		C07C												31-04		
			IPC	D	(ICS C07C							-08	[T A	1. 0	0700	215-	1.2		
			11.0	• `	[I,A]; C	07C0	215-	40 [
			ECL		C07C	215/	40;	C07C	215/										
CN	199	7620	IPC	I	CO7C] 00	I,C*]; B	01J0	031-	0 4		
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C07C0217-30 [I,A]
                 ECLA
                        C07C215/40; C07C215/08; C07C215/12; C07C217/30
 EP 1805131
                 IPCI
                        C07C0215-40 [I,A]; C07C0215-00 [I,C*]
                        C07C0215-00 [I,C]; C07C0215-40 [I,A]; C07C0215-08
                 IPCR
                        [I,A]; C07C0215-12 [I,A]; C07C0217-00 [I,C*];
                        C07C0217-30 [I,A]
                 ECLA
                        C07C215/40; C07C215/08; C07C215/12; C07C217/30
 JP 2007532525
                 IPCI
                        C07C0215-40 [I,A]; C07C0215-00 [I,C*]; C07C0311-03
                        [I,A]; C07C0311-00 [I,C*]
                 IPCR
                        C07C0215-00 [I,C]; C07C0215-40 [I,A]; C07C0215-08
                        |I,A|; C07C0215-12 |I,A|; C07C0217-00 |I,C*|;
                        C07C0217-30 [I,A]; C07C0311-00 [I,C]; C07C0311-03 [I,A]
                 FTERM
                       4H006/AA01; 4H006/AA03; 4H006/AB80
MX 2006011531
                 IPCI
                        B01J0031-02 [I,C*]; B01J0031-04 [I,C*]; C07C0215-40
                        [I,A]; C07C0215-00 [I,C*]
 IN 2006KN03208 TPCT
                        C07C0215-40 [ICM, 7]; C07C0215-00 [ICS, 7]
 KR 2007031302
                IPCI
                        C07C0215-40 [I,A]; C07C0215-00 [I,A]
 US 20070185330 IPCI
                        C07C0215-02 [I,A]; C07C0215-00 [I,C*]; C07D0211-02
                        [I,A]; C07D0211-00 [I,C*]
                NCL
                        546/184.000; 564/281.000
    MARPAT 143:386681
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O.S.

The present invention relates to ionic ligs, comprising an anion and a cation wherein the cation is a primary, secondary or tertiary ammonium ion containing a protonated nitrogen atom. The invention also provides processes for the manufacture of ionic ligs. For example, N,N-dimethylethanolammonium glycolate (I) was prepared by gradually adding glycolic acid to an alc. solution of N,N-dimethylethanolamine; after completion and neutralization, the cold alc. solution was filtered, solvent removed, then frozen in liquid nitrogen and lyophilized in vacuo. After gradually allowing the sample to warm to room temperature, 32.85 g (99% yield) of I as a pale yellow liquid was isolated. Preferred ionic ligs. contain ethanolammonium, diethanolammonium, N-butyldiethanolammonium, N,N-dimethylethanolammonium,

N-methylethanolammonium, N,N-di(methoxyethyl)ammonium and 1-(3-hydroxypropyl)putrescinium ions as cations.

amine acid; ammonium ionic liq prepn; primary ammonium ion prepn ionic lig; secondary ammonium ion prepn ionic lig; tertiary ammonium ion prepn ionic liq Oxidation

(enzymic; demonstration of application of ionic ligs. in enzymic oxidation of methanol to formaldehyde)

Green chemistry

Ionic liquids

(preparation and methods for manufacture of ionic ligs. containing protonated

primary, secondary or tertiary ammonium ions)

Quaternary ammonium compounds, preparation

RL: IMF (Industrial manufacture); NUU (Other use, unclassified); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)

(preparation and methods for manufacture of ionic liqs. containing protonated

primary, secondary or tertiary ammonium ions)

Acids, reactions

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation and methods for manufacture of ionic liqs. containing protonated

primary, secondary or tertiary ammonium ions)

Solvents

(preparation and methods for manufacture of ionic ligs. containing protonated

primary, secondary or tertiary ammonium ions for use as solvent in industrial and com. applications)

Amines, reactions

RL: RCT (Reactant); RACT (Reactant or reagent) (primary; preparation and methods for manufacture of ionic ligs. containing protonated primary, secondary or tertiary ammonium ions) Carboxvlic acids, uses Sulfonic acids, uses RL: NUU (Other use, unclassified); USES (Uses) (salts, anion component for ionic liquid; preparation and methods for manufacture of ionic ligs, containing protonated primary, secondary or tertiary ammonium ions) Amines, reactions RL: RCT (Reactant); RACT (Reactant or reagent) (secondary; preparation and methods for manufacture of ionic ligs. containing protonated primary, secondary or tertiary ammonium ions) Amines, reactions RL: RCT (Reactant); RACT (Reactant or reagent) (tertiary; preparation and methods for manufacture of ionic ligs. containing protonated primary, secondary or tertiary ammonium ions) 56-14-4, Succinate, uses 57-60-3, Pyruvate, uses 63-36-5, Salicylate, 71-47-6, Formate, uses 71-50-1, Acetate, uses 71-52-3, Hydrogen carbonate, uses 72-03-7, Propanoate, uses 74-81-7, Octanoate, uses 113-21-3, Lactate, uses 126-44-3, Citrate, uses 142-42-7, Fumarate, uses 191-33-7, Hexanoate, uses 338-70-5, uses 461-55-2, Butanoate, uses 666-14-8, uses 766-76-7, Benzoate, uses 769-61-9, Mandelate 3342-79-8, Nonanoate 3398-75-2 Decanoate 3715-17-1, Tartrate, uses 3812-32-6, Carbonate, uses 7563-37-3, Heptanoate 7631-42-7, Phenylacetate, uses 10023-74-2, Pentanoate, uses 12627-13-3, Silicate 14066-19-4, Hydrogen phosphate, uses 14066-20-7, Dihydrogen phosphate, uses 14265-44-2, Phosphate, 14477-72-6, Trifluoroacetate ion, uses 14797-55-8, Nitrate, uses 14808-79-8, Sulphate, uses 14874-70-5, Tetrafluoroborate 14996-02-2, Hydrogen sulfate, uses 16053-58-0, Methanesulfonate anion Chloride, uses 16919-18-9, Hexafluorophosphate 17121-12-9, Metaphosphate (P40124-) 20461-54-5, Iodide, uses 20938-62-9, Pantothenate 24959-67-9, Bromide, uses 37181-39-8, Trifluoromethanesulfonate 41824-21-9, Crotonate 44864-55-3 45048-62-2 49681-69-8, Hydrogen tartrate, uses 59561-61-4 86848-98-8 86848-99-9 97901-86-5 98837-98-0 130434-58-1 328238-56-8 866621-22-9 RL: NUU (Other use, unclassified); USES (Uses) (anion component for ionic liquid; preparation and methods for manufacture of ionic ligs. containing protonated primary, secondary or tertiary ammonium ions) 176158-74-0P RL: BSU (Biological study, unclassified); IMF (Industrial manufacture); NUU (Other use, unclassified); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses) (biodegrdn. anal. of ionic liquid; preparation and methods for manufacture of ionic ligs. containing protonated primary, secondary or tertiary ammonium ions) 22852-66-0, Ethanolamine conjugate acid 26265-71-4 36833-63-3 36833-64-4 65591-62-0 90578-97-5 866567-32-0 866567-33-1 866567-34-2 RL: NUU (Other use, unclassified); USES (Uses) (cation component for ionic liquid; preparation and methods for manufacture of ionic liqs. containing protonated primary, secondary or tertiary ammonium ions) 67-56-1, Methanol, reactions RL: RCT (Reactant); RACT (Reactant or reagent)

(demonstration of application of ionic ligs. in enzymic oxidation of

RL: SPN (Synthetic preparation); PREP (Preparation)

(demonstration of application of ionic liqs. in enzymic oxidation of methanol to formaldehyde)

2471-06-9P 2604-13-9P 2805-17-6P 3178-20-9P 4337-66-0P 7487-79-8P 16530-72-6P 16830-40-3P 5988-51-2P 17618-31-4P 17618-32-5P 17863-38-6P 18394-23-5P 20261-59-0P 20475-13-2P 20748-72-5P 21829-52-7P 23251-72-1P, Diethanolamine acetate 23349-61-3P 25859-29-4P 26764-31-8P 28098-03-5P 28129-21-7P, Diethanolamine hydrobromide 29194-47-6P 29867-71-8P 29867-72-9P 29867-75-2P 29868-00-6P 29868-01-7P 29870-14-2P 29870-15-3P 29870-18-6P 29870-19-7P 29870-25-5P 29870-26-6P 29870-27-7P 29870-29-9P 30718-92-4P 30933-06-3P 31086-83-6P 31889-13-1P 35423-90-6P 38491-11-1P 38739-74-1P 49753-18-6P 49753-20-0P 51264-32-5P 51276-44-9P 53226-35-0P 53562-95-1P 53926-87-7P 54300-24-2P 56669-87-5P 57117-29-0P 55756-39-3P 56409-18-8P 62036-98-0P 58937-21-6P 59101-30-3P 59866-70-5P 60395-28-0P 63517-71-5P 63517-72-6P 64601-03-2P 64601-04-3P 64601-14-5P 67303-52-0P 67384-57-0P 68141-00-4P 68141-46-8P 68391-54-8P. Diethanolamine formate 68568-51-4P 68815-69-0P 68833-69-2P 68860-57-1P 68945-90-4P 69362-00-1P 69362-01-2P 75478-96-5P 76788-90-4P 77534-69-1P 77534-73-7P 79266-74-3P 82801-62-5P 84176-56-7P 84110-42-9P 84145-30-2P 84145-60-8P 86683-38-7P 86683-39-8P 88331-27-5P 89855-93-6P 90000-02-5P 90434-46-1P 93882-26-9P 93882-27-0P 93942-28-0P 93942-29-1P 95332-67-5P 98005-86-8P 98837-33-3P 101901-23-9P 103079-19-2P 108067-35-2P 116033-27-3P 117472-14-7P 126050-30-4P 109962-24-5P 111318-69-5P 134227-25-1P 135691-53-1P 137360-57-7P 138036-64-3P 156814-01-6P 181180-62-1P 164460-12-2P 205490-53-5P 205490-69-3P 209052-82-4P 210040-56-5P 252280-99-2P 327156-58-1P 372169-26-1P 372169-30-7P 392292-52-3P 815574-85-7P 857086-60-3P 857086-63-6P 866567-31-9P 866567-31-9P 866567-35-3P 866567-36-4P 866567-37-5P 866567-38-6P 866567-39-7P 866567-40-0P 866567-41-1P 866567-42-2P 866567-43-3P 866567-44-4P 866567-45-5P 866567-46-6P 866567-47-7P 866567-48-8P 866567-49-9P 866567-50-2P 866567-51-3P 866567-52-4P 866567-53-5P 866567-54-6P 866567-55-7P 866567-56-8P 866567-57-9P 866567-58-0P 866567-59-1P 866567-60-4P 866567-61-5P 866567-62-6P 866567-63-7P 866567-65-9P 866567-67-1P 866567-69-3P 866567-70-6P 866567-71-7P 866567-72-8P 866567-73-9P 866567-74-0P 866567-75-1P 866567-76-2P 866567-77-3P 866567-78-4P 866567-79-5P 866567-80-8P 866567-81-9P 866567-82-0P 866567-83-1P 866567-84-2P 866567-85-3P 866567-86-4P 866567-87-5P 866567-88-6P 866567-89-7P 866567-90-0P 866567-91-1P 866567-92-2P 866567-93-3P 866567-94-4P 866567-95-5P 866567-96-6P 866567-97-7P 866567-98-8P 866567-99-9P 866568-00-5P 866568-01-6P 866568-02-7P 866568-03-8P 866568-04-9P 866568-05-0P 866568-06-1P 866568-07-2P 866568-08-3P 866568-10-7P 866568-11-8P 866568-09-4P 866568-13-0P 866568-16-3P 866568-12-9P 866568-15-2P 866568-17-4P 866568-19-6P 866568-20-9P 866568-21-0P 866568-22-1P 866568-18-5P 866568-23-2P 866568-24-3P 866568-25-4P 866568-26-5P 866568-27-6P 866568-28-7P 866568-29-8P 866568-30-1P 866568-31-2P 866568-32-3P 866568-33-4P 866568-34-5P 866568-35-6P 866568-36-7P 866568-37-8P 866568-41-4P 866568-38-9P 866568-39-0P 866568-40-3P 866568-42-5P 866568-43-6P

RL: IMF (Industrial manufacture); NUU (Other use, unclassified); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)

(preparation and methods for manufacture of ionic liqs. containing protonated $% \left(1\right) =\left(1\right) \left(1\right) \left($

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	trial manufactu:		use, unclassif.	ied); SPN
	paration); PREP		USES (Uses)	
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(Synthetic preparation); FREF (Preparation); USES (USES)
(preparation and methods for manufacture of ionic liqs. containing protonated

PLOC	onacca				
	primary, se	condary or tert	iary ammonium	ions)	
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     RL: IMF (Industrial manufacture); NUU (Other use, unclassified); SPN
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        (preparation and methods for manufacture of ionic ligs. containing
protonated
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     79-14-1, Glycolic acid, reactions 102-79-4, N-Butyldiethanolamine
     108-01-0, N.N-Dimethylethanolamine 82113-65-3
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (preparation and methods for manufacture of ionic ligs. containing
protonated
       primary, secondary or tertiary ammonium ions)
             THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD
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L28 ANSWER 17 OF 21 CAPLUS COPYRIGHT 2009 ACS on STN
     2005:561949 CAPLUS
DN
     143:229956
    Entered STN: 30 Jun 2005
    Synthesis and Characterization of Organometallic Ionic
     Liquids and a Heterometallic Carbene Complex Containing the
     Chromium Tricarbonyl Fragment
AU
    Moret, Marc-Etienne; Chaplin, Adrian B.; Lawrence, Adrien K.; Scopelliti,
     Rosario; Dyson, Paul J.
    Institut des Sciences et Ingenierie Chimiques, EPFL-BCH, Lausanne,
    CH-1015, Switz.
SO
    Organometallics (2005), 24(16), 4039-4048
    CODEN: ORGND7; ISSN: 0276-7333
PB
    American Chemical Society
DT
    Journal
LA
    English
CC
    29-11 (Organometallic and Organometalloidal Compounds)
    Section cross-reference(s): 75
    CASREACT 143:229956
OS
AB
    Direct reaction between [Cr(CO)6] and arenes with ionic substituents
     affords the corresponding arene-Cr tricarbonvl complexes,
     [Cr(CO)3(arene)], in only modest (4-32%) yield. In contrast, these
     complexes can be prepared in pure form in excellent yield from the reaction
     of [Cr(CO)3(n6-C6H5CH2Br)] with, for example, N-methylimidazole. The
     structures of [Cr(CO)3(\eta6-C6H5CH2MIM)]Br(MIM = 3-methylimidazolium),
     [Cr(CO)3(\eta6-C6H5CH2MMIM)]Br(MMIM = 2,3-dimethylimidazolium), and
     [Cr(CO)3(n6-C6H5CH2NMe2Me2OH)]Br were established by x-ray diffraction
     anal. Subsequent exchange of the bromide anion for Tf2N- affords new
     organometallic salts with m.ps. <70°. Reaction of the bromide
     salts includes tosylation of [Cr(CO)3(η6-C6H5CH2NMe2Me2OH)]Br to
     afford [Cr(CO)3(n6-C6H5CH2NMe2(CH2)2OTs)]Br and the formation of the
     heterometallic carbene complex [Ru(η6-p-cymene)Cl2{C4H5N2CH2Ph-η6-
     Cr(CO)3}]. Both compds. were characterized in the solid state by x-ray
    diffraction.
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RE

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ΤI

CS

chromium tricarbonyl derivatized ionic liq prepn; benzylimidazolium chromium tricarbonyl deriv prepn structure reaction; ruthenium chromium heterometallic carbene benzylimidazole deriv prepn structure; crystal

structure chromium tricarbonyl benzylimidazolium heterometallic ruthenium benzylimidazole carbene; mol structure chromium tricarbonyl benzylimidazolium heterometallic ruthenium benzylimidazole carbene

Crystal structure

Molecular structure

(of chromium tricarbonyl benzylimidazolium organometallic ionic ligs. and chromium-ruthenium heterometallic benzylimidazole carbene complex)

Ionic liquids (organometallic; preparation and structure of chromium tricarbonyl

benzylimidazolium-containing ionic ligs, and of chromium-ruthenium heterometallic benzylimidazole carbene complex)

Aromatic hydrocarbons, reactions

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation and structure of chromium tricarbonyl

benzylimidazolium-containing

ionic liqs. and of chromium-ruthenium heterometallic benzylimidazole carbene complex)

862999-66-4P 862999-67-5P 862999-68-6P

RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(crystal structure; preparation and structure of chromium tricarbonyl benzylimidazolium-containing ionic ligs, and of chromium-ruthenium heterometallic benzylimidazole carbene complex)

862999-72-2P 862999-74-4P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (crystal structure; preparation and structure of chromium tricarbonyl benzylimidazolium-containing ionic liqs. and of chromium-ruthenium heterometallic benzylimidazole carbene complex)

108-01-0, 2-(Dimethylamino)ethanol 616-47-7, N-Methylimidazole 637-59-2 1739-84-0, 1,2-Dimethylimidazole 7221-41-2 13007-92-6, Chromium hexacarbonyl 52462-29-0 65039-11-4 191352-85-9 862999-80-2 862999-81-3

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation and structure of chromium tricarbonyl

benzylimidazolium-containing

ionic liqs. and of chromium-ruthenium heterometallic benzylimidazole carbene complex)

500996-04-3P 862999-75-5P 862999-76-6P 862999-77-7P 862999-78-8P 862999-79-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and structure of chromium tricarbonyl benzylimidazolium-containing

ionic liqs. and of chromium-ruthenium heterometallic benzylimidazole carbene complex)

862999-57-3P 862999-59-5P 862999-61-9P 862999-63-1P 862999-65-3P 862999-69-7P 862999-70-0P 862999-71-1P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation and structure of chromium tricarbonyl

benzylimidazolium-containing

ionic ligs. and of chromium-ruthenium heterometallic benzylimidazole carbene complex)

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L28 ANSWER 18 OF 21 CAPLUS COPYRIGHT 2009 ACS on STN
AN
   2004:753469 CAPLUS
DN
   141:280342
ED
    Entered STN: 16 Sep 2004
TΙ
    Polymer particle dispersions, electrolytes and quasi-solid electrolytes
    comprising same dispersions, and batteries employing same quasi-solid
    electrolytes
IN
    Nagano, Toshiaki; Ogawa, Tetsuo
PA
    Kansai Paint Co., Ltd., Japan
SO
    Jpn. Kokai Tokkvo Koho, 15 pp.
    CODEN: JKXXAF
    Patent.
LA
    Japanese
TC:
    ICM C08F002-12
    ICS C08F012-00; C08F020-00; H01B001-06; H01M008-02; H01M010-40;
         H01M014-00
    52-2 (Electrochemical, Radiational, and Thermal Energy Technology)
    Section cross-reference(s): 38, 76
FAN.CNT 1
    PATENT NO.
                       KIND
                                          APPLICATION NO.
                                                                DATE
                              DATE
                       ----
    JP 2004256711
                        A
                               20040916 JP 2003-50180
                                                                20030227
PRAI JP 2003-50180
                               20030227
CLASS
PATENT NO. CLASS PATENT FAMILY CLASSIFICATION CODES
JP 2004256711 ICM
                       C08F002-12
                ICS
                       C08F012-00; C08F020-00; H01B001-06; H01M008-02;
                       H01M010-40; H01M014-00
                IPCI
                       C08F0002-12 [ICM.71; C08F0012-00 [ICS.71; C08F0020-00
                       [ICS, 7]; H01B0001-06 [ICS, 7]; H01M0008-02 [ICS, 7];
                       H01M0010-40 [ICS, 7]; H01M0010-36 [ICS, 7, C*];
                       H01M0014-00 [ICS,7]
                       C08F0002-12 [I,A]; C08F0002-12 [I,C*]; C08F0012-00
                TPCR
                       [I,A]; C08F0012-00 [I,C*]; C08F0020-00 [I,A];
                       C08F0020-00 [I,C*]; H01B0001-06 [N,A]; H01B0001-06
                       [N.C*1; H01M0008-02 [N,A]; H01M0008-02 [N,C*];
                       H01M0010-36 [N,C*]; H01M0010-40 [N,A]; H01M0014-00
                        [N,A]; H01M0014-00 [N,C*]
                FTERM 4J011/AA05; 4J011/KA01; 4J011/KA15; 4J011/KB08;
                       4J011/KB19; 4J011/KB28; 4J011/KB29; 4J011/KB30;
                       5G301/CA30; 5G301/CD01; 5H026/AA06; 5H026/HH01;
                       5H026/HH05; 5H026/HH06; 5H029/AJ06; 5H029/AM16;
                       5H029/DJ09; 5H029/HJ01; 5H029/HJ05; 5H029/HJ20;
                       5H032/AA06; 5H032/AS16; 5H032/EE01; 5H032/EE07;
                       5H032/EE16; 5H032/HH01; 5H032/HH04; 5H032/HH08
   Polymer particle dispersions comprise ionic liqs. as disperse media. Also
AB
    claimed are electrolytes with elec. conductivity between (1 + 10-9) and (1
```

+ 107) S/cm. The (quasi-solid) electrolytes are suitable for

- dye-sensitized solar cells, secondary lithium batteries, and fuel cells. ST polymer particle dispersion ionic lid medium; electrolyte polymer particle dispersion ionic lid; quasi solid electrolyte polymer particle dispersion ionic liq; lithium battery quasi solid electrolyte ionic lid disperse medium; dye sensitized battery quasi solid electrolyte ionic lid dispersion
- IT Secondary batteries

(lithium; polymer particle dispersions containing ionic liquid disperse media, for (quasi-solid) electrolytes and batteries)

IT Electrolytes

Ionic liquids

(polymer particle dispersions containing ionic liquid disperse media, for (quasi-solid) electrolytes and batteries)

IT Solar cells

(quasi-solid electrolytes; polymer particle dispersions containing ionic liquid disperse media, for (quasi-solid) electrolytes and batteries)

IT Battery electrolytes

(quasi-solid; polymer particle dispersions containing ionic liquid disperse media, for (quasi-solid) electrolytes and batteries)

IT 64-19-7DP, Acetic acid, reaction products with cresol novolak epoxy resins and amines, polymer with acrylic monomers 100-42-5DP, Styrene, polymers with cresol novolak epoxy resins quaternary ammonium salts, polymer with acrylic monomers 108-01-0DP, N,N-Dimethylaminoethanol, reaction products with cresol novolak epoxy resins and acetic acid, polymer with acrylic monomers 606-59-3DP, 1,6-Hexanediol dimethacrylate, polymers with cresol novolak epoxy resins quaternary ammonium salts, polymer with acrylic monomers 78949-77-6P, 1,6-Hexanediol dimethacrylate-styrene copolymer 181140-08-9DP, ESCN 195 acrylate, reaction products with amines and acetic acid, polymer with acrylic monomers 757973-29-8P 757973-30-1P 757973-31-9

RL: DEV (Device component use); IMF (Industrial manufacture); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses) (crosslinked, particles; polymer particle dispersions containing ionic

liquid

disperse media, for (quasi-solid) electrolytes and batteries)

RL: DEV (Device component use); TEM (Technical or engineered material use); USES (Uses)

(ionic liqs.; polymer particle dispersions containing ionic liquid disperse media, for (quasi-solid) electrolytes and batteries)

- L28 ANSWER 19 OF 21 CAPLUS COPYRIGHT 2009 ACS on STN
- AN 2004:580287 CAPLUS
- DN 141:270457
- ED Entered STN: 21 Jul 2004
- TI Phosphazene-Based Ionic Liquids: Synthesis, Temperature-Dependent Viscosity, and Effect as Additives in Water Lubrication of Silicon Nitride Ceramics
- AU Omotowa, Bamidele A.; Phillips, Benjamin S.; Zabinski, Jeffery S.; Shreeve, Jean'ne M.
- CS Department of Chemistry, University of Idaho, Moscow, ID, 83844-2343, USA SO Inorganic Chemistry (2004), 43(17), 5466-5471
- CODEN: INOCAJ; ISSN: 0020-1669
- PB American Chemical Society
- DT Journal
- LA English
- CC 78-8 (Inorganic Chemicals and Reactions)
- Section cross-reference(s): 29, 57, 65
- OS CASREACT 141:270457
- AB Phosphazene rings with alkoxy chain substituents, N3P3(R)(R')5 [R = allyloxy, R' = 2-(dimethylamino)ethoxy (1); R = R' = 2-(dimethylamino)ethoxy (2); R = R' = 4-pyridylmethoxy (3)] and N4P4R8 [R

= 3-(dimethylamino)propoxy] (4) were synthesized and quaternized at the substituent nitrogen by treatment with Me iodide at 35° over 3-6 h to give polyiodo salts (5-8), resp. Subsequent metathesis with LiN(SO2CF3)2 gave the resp. ionic salts (9-12) or, with NaBF4, 7 gave (13). The amide salts, 9-12, were viscous liqs. with pour points at 55-100°, and the tetrafluoroborate salt, 13, was a solid, m.p. 168°. The compns. of 2 and 5-13 were confirmed by elemental anal. and spectroscopic methods. Compds. 1, 2, and 4 were viscous liqs. (d25 =1.67 g cm-3; $\eta_{25} = 0.76-1.56$ mPa s-1) with pour points at .apprx.15°. The solid polyquaternary salts, 5-8, melted at 130-194°. The ionic liqs., 9-12, had an average d. of .apprx.1.73 g cm-3 at 25°, and viscosities (25°) ranged between 68.3 and 139.2 mPa s-1. A plot of the viscosities of 9-12 vs. temperature revealed an almost linear correlation between 55 and 120°. Friction and wear properties of water with 0.25% of 9-12 as boundary lubricant additives were evaluated on Si3N4/Si3N4 ceramic interfaces. The most significant observation is that they caused a decrease in the running-in period. alkoxy phosphazene ionic liq prepn viscosity silicon nitride lubricant; cyclophosphazene alkoxy ionic liq prepn viscosity silicon nitride lubricant Lubrication (boundary; preparation of trimethylammonioalkoxy- and methylpyridiniomethoxy-substituted phosphazene-based ionic ligs., temperature-dependent viscosity, and effect as additives in water lubrication of silicon nitride ceramics) Density Ionic liquids Pour point Viscosity (preparation of trimethylammonioalkoxy- and methylpyridiniomethoxy-substituted phosphazene-based ionic ligs., temperature-dependent viscosity, and effect as additives in water lubrication of silicon nitride ceramics) Cyclophosphazenes RL: MOA (Modifier or additive use); PEP (Physical, engineering or chemical process); PRP (Properties); PYP (Physical process); SPN (Synthetic preparation); PREP (Preparation); PROC (Process); USES (Uses) (preparation of trimethylammonioalkoxy- and methylpyridiniomethoxy-substituted phosphazene-based ionic ligs., temperature-dependent viscosity, and effect as additives in water lubrication of silicon nitride ceramics) Lubricants (water-based; preparation of trimethylammonioalkoxy- and methylpyridiniomethoxy-substituted phosphazene-based ionic ligs., temperature-dependent viscosity, and effect as additives in water lubrication of silicon nitride ceramics) 756526-84-8P 756526-86-0P 756526-88-2P 756526-90-6P RL: MOA (Modifier or additive use); PEP (Physical, engineering or chemical process); PRP (Properties); PYP (Physical process); SPN (Synthetic preparation); PREP (Preparation); PROC (Process); USES (Uses) (preparation of trimethylammonioalkoxy- and methylpyridiniomethoxy-substituted phosphazene-based ionic liqs., temperature-dependent viscosity, and effect as additives in water lubrication of silicon nitride ceramics) 108-01-0, N,N-Dimethylamino-2-ethanol 940-71-6. Hexachlorotriphosphazene 2950-45-0, Octachlorotetraphosphazene

3179-63-3, N,N-Dimethylamino-3-propanol 89490-86-8,

```
(Allyloxy)pentachlorotriphosphazene
                                           90076-65-6, Lithium
     bis(trifluoromethylsulfonyl)amide
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (preparation of trimethylammonioalkoxy- and
        methylpyridiniomethoxy-substituted phosphazene-based ionic liqs.,
        temperature-dependent viscosity, and effect as additives in water
lubrication
        of silicon nitride ceramics)
                                                  756526-78-0P
     211054-44-3P 211913-55-2P
                                    756526-77-9P
                                                                  756526-79-1P
     756526-80-4P
                   756526-81-5P
                                   756526-82-6P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (preparation of trimethylammonioalkoxy- and
        methylpyridiniomethoxy-substituted phosphazene-based ionic liqs.,
        temperature-dependent viscosity, and effect as additives in water
lubrication
        of silicon nitride ceramics)
     756526-91-7P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (preparation of trimethylammonioalkoxy- and
        methylpyridiniomethoxy-substituted phosphazene-based ionic ligs.,
        temperature-dependent viscosity, and effect as additives in water
lubrication
        of silicon nitride ceramics)
     12033-89-5, Silicon nitride (Si3N4), uses
     RL: TEM (Technical or engineered material use); USES (Uses)
        (preparation of trimethylammonioalkoxy- and
        methylpyridiniomethoxy-substituted phosphazene-based ionic liqs.,
        temperature-dependent viscosity, and effect as additives in water
lubrication
        of silicon nitride ceramics)
RE.CNT 31
             THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD
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RE

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L28 ANSWER 20 OF 21 CAPLUS COPYRIGHT 2009 ACS on STN
AN
    2004:328162 CAPLUS
DN
    141:313871
ED
    Entered STN: 22 Apr 2004
    Room temperature ionic liquids - new choline
    derivatives
AII
     Pernak, J.; Chwala, P.; Syguda, A.
CS
     Faculty of Chemical Technology, Poznan University of Technology, Poznan,
     60-965, Pol.
SO
     Polish Journal of Chemistry (2004), 78(4), 539-546
     CODEN: PJCHDQ; ISSN: 0137-5083
PB
     Polish Chemical Society
DT
    Journal
LA
     English
CC
     23-4 (Aliphatic Compounds)
os
    CASREACT 141:313871
AB
    New room temperature ionic ligs. R10(CH2)2N+Me2CH2OR2 -N(SO2CF3)2 (I, R1 = H,
     COMe, R2 = Et, n-Pr, C10H21, etc.) - choline derivs. were prepared by
     Menschutkin reaction with alkyl chloromethyl ethers and anion changed to
     bis(trifluoromethylsulfonyl)amide ion. The newly obtained
     butoxymethyl(2-hydroxyethyl)dimethylammonium
     bis(trifluoromethanesulfonyl)amide I (R1 = H, R2 = n-Bu) was successfully
     tested as a solvent for O-acylation of deanol with acid chlorides in a
     two-phase reaction system. The ionic liquid-catalyst system was recycled
     and reused.
ST
    room temp ionic liq prepn solvent acylation deanol;
     alkoxymethylhydroxyethylammonium trifluoromethanesulfonylamide ionic liq
     prepn solvent acylation deanol; green chem
     alkoxymethylhydroxyethylammonium trifluoromethanesulfonylamide ionic lig
     solvent; ammonium trifluoromethanesulfonylamide alkoxymethylhydroxyethyl
     ionic liq prepn solvent acylation deanol
    Esterification
       Ionic liquids
        (preparation of alkoxymethyl(hydroxyethyl)dimethylammonium
        trifluoromethanesulfonylamides as room temperature ionic ligs. and use as
        solvent for O-acvlation of deanol)
     RL: CAT (Catalyst use); RCT (Reactant); SPN (Synthetic preparation); PREP
     (Preparation); RACT (Reactant or reagent); USES (Uses)
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(preparation of alkoxymethy1(hydroxyethy1)dimethylammonium trifluoromethanesulfonylamides as room temperature ionic ligs. and use as solvent for O-acylation of deanol) T 767320-88-7P Rl: NUU (Other use, unclassified); SPN (Synthetic preparation); PREP (Preparation); USES (Uses) (preparation of alkoxymethy1(hydroxyethy1)dimethylammonium trifluoromethanesulfonylamides as room temperature ionic ligs. and use as

T 98-88-4, Bensoyl chloride 108-01-0, Deanol 111-64-8, Octanoyl chloride 112-13-0, Decanoyl chloride 2351-69-1, Chloromethyl butyl ether 3188-13-4, Chloromethyl ethyl ether 3587-57-3, Chloromethyl propyl ether 13497-61-5, Chloromethyl dodecyl ether 19416-65-0, Chloromethyl pentyl ether 24566-90-3, Chloromethyl octyl ether 24566-91-4, Chloromethyl nonyl ether 24566-92-5, Chloromethyl decyl ether 24566-93-6, Chloromethyl undecyl ether 39979-92-5, Chloromethyl hexyl ether 49791-06-2, Chloromethyl heptyl ether RL: RCT (Reactant); RACT (Reactant); RACT (Reactant)

(preparation of alkoxymethyl(hydroxyethyl)dimethylammonium

solvent for O-acylation of deanol)

trifluoromethanesulfonylamides as room temperature ionic liqs. and use as solvent for O-acylation of deanol)

- IT 1421-89-2P, 2-(Dimethylamino)ethyl acetate 38954-45-9P 38954-46-0P 38954-47-1P 38954-48-2P 38954-49-3P 646068-98-6P 646069-00-3P 646069-01-4P 646069-02-5P 767320-70-7P 767320-71-8P 767320-76-3P 767320-77-4P 767320-78-5P 767320-79-6P 767320-89-9P 767320-81-0P
 - 767320-82-1P 767320-83-2P 767320-84-3P 767320-85-4P RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 - (preparation of alkoxymethyl(hydroxyethyl)dimethylammonium

trifluoromethanesulfonylamides as room temperature ionic liqs. and use as solvent for O-acylation of deanol)

- IT 90076-65-6
 - RL: RGT (Reagent); RACT (Reactant or reagent)
 - (preparation of alkoxymethyl(hydroxyethyl)dimethylammonium

trifluoromethanesulfonylamides as room temperature ionic liqs. and use as solvent for O-acylation of deanol)

- 767320-75-2P IΤ 2208-05-1P 36609-93-5P 129320-08-7P 767320-73-0P 767320-86-5P 767320-89-8P 767320-90-1P 767320-91-2P 767320-92-3P 767320-93-4P 767320-94-5P 767320-95-6P 767320-96-7P 767320-98-9P 767321-04-0P 767321-06-2P 767321-08-4P 767321-00-6P 767321-02-8P 767321-10-8P 767321-12-0P 767321-14-2P 767321-16-4P RL: SPN (Synthetic preparation); PREP (Preparation)
 - (preparation of alkoxymethyl(hydroxyethyl)dimethylammonium

trifluoromethanesulfonylamides as room temperature ionic liqs. and use as solvent for O-acylation of deanol)

- RE.CNT 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD RE
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- L28 ANSWER 21 OF 21 CAPLUS COPYRIGHT 2009 ACS on STN
- AN 2004:56092 CAPLUS
- DN 140:270820
- ED Entered STN: 23 Jan 2004
- TI Triazine-Based Polyfluorinated Triquaternary Liquid Salts: Synthesis, Characterization, and Application as Solvents in Rhodium(I)-Catalyzed Hydroformylation of 1-Octene
- AU Omotowa, Bamidele A.; Shreeve, Jean'ne M.
- CS Department of Chemistry, University of Idaho, Moscow, ID, 83844-2343, USA

- SO Organometallics (2004), 23(4), 783-791 CODEN: ORGND7; ISSN: 0276-7333
- PB American Chemical Society
- DT Journal
- LA English
- CC 28-19 (Heterocyclic Compounds (More Than One Hetero Atom))
 - Section cross-reference(s): 23, 67
- OS CASREACT 140:270820
- AB Silvlation of N-(2-hydroxyethyl)imidazole, HOCH2CH2Im (1), with hexamethyldisilazane gave N-(2-trimethylsilyloxyethyl)imidazole, Me3SiOCH2CH2Im (2), which underwent quaternization reactions with the alkyl halides and gave three new N-(trimethylsilyloxyethyl) imidazolium halides, Me3SiOCH2CH2Im+RX-, where Im+ = imidazolium and R/X = Me/I (3), CH2CH2F/Br (4), and CH2CH2CF3/I (5). The Et ether, formed from 1 and Et bromide was quaternized with CF3CH2CH2I followed by anion exchange with LiN(SO2CF3)2 to obtain [CF3CH2CH2Im+CH2CH2OEt N(SO2CF3)2-] (8). The metathesis reactions of 3-5 with cyanuric fluoride in acetonitrile at 25° gave tris[2-(N'-alkylimidazolium)ethoxy]triazine trihalides, N3C3(OCH2CH2Im+RX-)3, where R/X = Me/I (9), CH2CH2F/Br (10), and CH2CH2CF3/I (11). Two neutral trimeric compds., N3C3(OCH2CH2Im)3 (12) and N3C3(OCH2CH2NMe2)3 (14), were prepared from reactions of cyanuric fluoride and Me3SiOCH2CH2NMe2 or 2, resp. The quaternization of 12 with MeI gave tris[oxoethyl(trimethyl)ammonium]triazine, N3C3(OCH2CH2N+Me3I-)3 (14). Subsequent exchange of the halides in 9-11 and N3C3(OCH2CH2N+Me3I-)3 (15) with the weakly coordinating anions of AgOSO2CF3, LiN(SO2CF3)2, AgNO3, or AgClO4 resulted in new triquaternary salts that were characterized by NMR, elemental analyses, and, for some of the compds., mass spectroscopy. Phys. (m.p. and d.) and thermal properties of compds. prepared were determined with differential scanning calorimeter (DSC) and thermogravimetric analyzer (TGA). In Rh(I)-catalyzed hydroformylation of 1-octene, with Ph2P(NMPBTA) [NMPBTA = N-methylpyridinium bis(trifluoromethanesulfonyl)amide] as ligand, the turnover frequency (TOF), conversion, isomer selectivity (n/i), and recyclability were compared when triquaternary salts or monoquaternary were used as solvents
- 8 as solvent. Striazine polyfluorinated triquaternary liq salt prepn solvent; rhodium catalyzed hydroformylation octene polyfluorinated triazine triquaternary liq solvent; thermogravimetric thermal property polyfluorinated triazine triquaternary liq salt solvent
- IT Solvents
 - (ionic ligs.; synthesis, characterization, and application of triazine-based polyfluorinated triquaternary liquid salts as solvents in rhodium-catalyzed hydroformylation of octene)

in the biphasic hydroformylation process. A change of metal/ligand ratio resulted in significant increase of n/i selectivity, but was marginal with

- IT Quaternary ammonium compounds, preparation
 - RL: NUU (Other use, unclassified); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
 - (solvents; synthesis, characterization, and application of triazine-based polyfluorinated triquaternary liquid salts as solvents in rhodium-catalyzed hydroformylation of octene)
- IT Differential scanning calorimetry Hydroformylation catalysts
 - Ionic liquids
 - Tonic IIquius
 - Thermal properties
 - Thermogravimetric analysis
 - (synthesis, characterization, and application of triazine-based polyfluorinated triquaternary liquid salts as solvents in
- rhodium-catalyzed hydroformylation of octene) IT 673686-75-4P 673687-58-6P 673687-65-5P
- RL: NUU (Other use, unclassified); PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent);

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USES (Uses)
        (solvent, thermal properties; synthesis, characterization, and
        application of triazine-based polyfluorinated triquaternary liquid salts
        as solvents in rhodium-catalyzed hydroformylation of octene)
ΤТ
     14874-82-9, (Acetylacetonato)dicarbonylrhodium
     RL: CAT (Catalyst use); USES (Uses)
        (synthesis, characterization, and application of triazine-based
        polyfluorinated triguaternary liquid salts as solvents in
        rhodium-catalyzed hydroformylation of octene)
     673687-18-8P
     RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP
     (Preparation); RACT (Reactant or reagent)
        (synthesis, characterization, and application of triazine-based
        polyfluorinated triquaternary liquid salts as solvents in
        rhodium-catalyzed hydroformylation of octene)
     107-07-3, 2-Chloroethanol, reactions 108-01-0,
     2-N, N-Dimethylaminoethanol 111-66-0, 1-Octene
                                                      288-32-4, Imidazole,
               460-37-7, 3,3,3-Trifluoropropyl iodide 675-14-9, Cyanuric
     reactions
     fluoride
                762-49-2, 1-Bromo-2-fluoroethane 1079-66-9,
     Chlorodiphenylphosphine 3430-13-5, 5-Bromo-2-methylpyridine
     90076-65-6, Lithium bis(trifluoromethylsulfonyl)amide
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (synthesis, characterization, and application of triazine-based
        polyfluorinated triquaternary liquid salts as solvents in
        rhodium-catalyzed hydroformylation of octene)
     1615-14-1P, 1-(2-Hydroxyethyl)imidazole 16654-64-1P 132682-77-0P
     197712-86-0P
                  673686-35-6P 673686-67-4P 673687-75-7P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (synthesis, characterization, and application of triazine-based
        polyfluorinated triquaternary liquid salts as solvents in
        rhodium-catalyzed hydroformylation of octene)
                        7786-29-0P, 2-Methyloctanal
     124-19-6P, Nonanal
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (synthesis, characterization, and application of triazine-based
        polyfluorinated triquaternary liquid salts as solvents in
        rhodium-catalyzed hydroformylation of octene)
     673687-83-7P
     RL: CAT (Catalyst use); RCT (Reactant); SPN (Synthetic preparation); PREP
     (Preparation); RACT (Reactant or reagent); USES (Uses)
        (thermal properties; synthesis, characterization, and application of
        triazine-based polyfluorinated triguaternary liquid salts as solvents in
       rhodium-catalyzed hydroformylation of octene)
     132684-26-5P
                  673686-41-4P 673686-48-1P
                                                 673686-55-0P
                                                                673686-81-2P
     673686-87-8P
                   673686-90-3P 673686-95-8P
                                                 673687-12-2P
                                                                673687-24-6P
     673687-32-6P
                  673687-39-3P 673687-46-2P 673687-50-8P
     RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP
     (Preparation): RACT (Reactant or reagent)
        (thermal properties; synthesis, characterization, and application of
        triazine-based polyfluorinated triquaternary liquid salts as solvents in
        rhodium-catalyzed hydroformylation of octene)
RE.CNT 59
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